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Integration des interaktiven Graphikpaketes »GDDM Interactive Chart Utility« in die menügeführte SAS-Benutzeroberfläche WAMASTAT

Wolfgang Schreiner

Zusammenfassung

Die vom System WAMASTAT gebotene Benutzeroberfläche ermöglicht den interaktiven Aufruf mehrerer SAS-Prozeduren, ohne daß der Benutzer syntaktisch richtige SAS-Befehle eingeben muß. Die bisher verfügbaren Funktionen von WAMASTAT wurden nun um eine spezielle Graphikfunktion erweitert, die es erlaubt, jedes SAS-Datenset in das interne Format der IBM GDDM Interactive Chart Utility (ICU) zu transferieren und dort weiter zu bearbeiten. Grundlage dafür ist eine an der 2. Chirurgischen Universitätsklinik entwickelte SAS-Prozedur (PROC SASICU), die in jedem SAS-Job mit der gewohnten Syntax aufgerufen werden kann, die Daten in die ICU transferiert und den Benutzer direkt in das Hauptmenü der ICU führt. Durch die Integration von PROC SASICU bietet WAMASTAT nun interaktive Graphik für jedes WAMASTAT-Datenset, aber auch für Ergebnisse von Statistikprozeduren, deren Aufruf durch WAMASTAT unterstützt wird.

Summary

WAMASTAT, a menu driven user front-end for SAS, offers interactive invocation of several SAS procedures, rendering the specification of syntactically correct SAS control statements unnecessary on the part of the user. On top of the WAMASTAT functions available so far a menu branch has been added to transfer arbitrary SAS data sets to the IBM GDDM Interactive Chart Utility (ICU) where the graphics may be modified interactively. This feature is based upon an SAS procedure (PROC SASICU) developed at the 2nd Surgical University Clinic. This procedure converts SAS data to GDDM format and transfers control to the main menu of the ICU. Following the integration of PROC SASICU, WAMASTAT now offers interactive graphics, not only for every WAMASTAT data set but also for the results of SAS procedures supported by WAMASTAT.

1. Einleitung

SAS (Statistic Analysis System) ist eines der bekanntesten und besten integrierten Pakete zur Datenerfassung, statistischen Analyse und graphischen Aufbereitung (6, 7, 8). Die Benutzung erfordert jedoch die Bedienung eines Editors sowie die Kenntnis der SAS control language. Für den Anwender wird es daher notwendig, Handbücher zu verwenden sowie syntaktische Fehler zu suchen und zu korrigieren. Diese Anforderungen stellen vielfach eine unzumutbare Mehrbelastung für klinisch tätige Ärzte dar und führten zur Entwicklung der menügesteuerten Benutzeroberfläche WAMASTAT, die im Multiple-choice-Verfahren alle notwendigen Informationen vom Benutzer erfragt, danach ein syntaktisch korrektes SAS-Programm erzeugt, dieses exekutiert und die Ergebnisse darstellt (1, 2, 4, 5).

Während für jede Statistikprozedur die möglichen Optionen relativ leicht standardisierbar sind und zudem vor dem Aufruf angegeben werden können, ist dies für graphische Darstellungen nicht der Fall; hier kann die optische Wirkung erst beim Betrachten der Graphik beurteilt werden und macht interaktive Modifikationen erforderlich. Gerade diese Funktion wird aber von den SAS-Graphikprozeduren (GPLOT, GCHART etc.) nicht geboten. Aus diesem Grund waren bisher nur

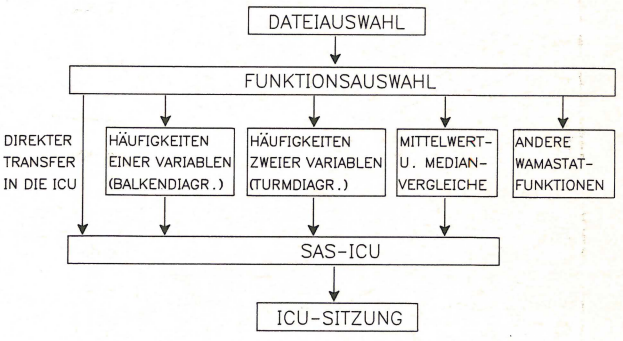

Abb. 1. Einbindung des Datentransfers in die ICU innerhalb des Systems WAMASTAT. Zusätzlich zu den bisher vorhandenen WAMASTAT-Funktionen (subsumiert in dem rechten Kasten »andere WAMASTAT-Funktionen«) wurde der »Direkte Transfer in die ICU« als neue Funktion eingebaut und ist menügesteuert abrufbar (siehe Abb. 2). Außerdem können die Ergebnisse anderer Statistikprozeduren (Häufigkeiten, Mittelwerte) automatisch nach ICU übertragen werden. Endpunkt des Datentransfers ist eine ICU-Sitzung, bei der alle Daten aus WAMASTAT für die interaktive graphische Bearbeitung zur Verfügung stehen

relativ einfache SAS-Graphiken über die Benutzeroberfläche WAMASTAT unterstützbar. Wollte man speziellere Darstellungen erreichen, mußte man auf die echte SAS-Programmierung zurückgreifen und sich die dazu nötigen Kenntnisse aneignen.

Durch die Erstellung der selbst entwickelten SAS-Prozedur PROC SASICU können jedoch SAS-Daten in die IBM GDDM Interactive Chart Utility (ICU) (3) transferiert werden und stehen dort zur menügesteuerten Modifikation zur Verfügung. Wie andere SAS-Prozeduren erfordert jedoch auch PROC SASICU einen syntaktisch korrekten Aufruf in der SAS control language (korrekte Variablenlisten etc). PROC SASICU wurde nun in das System WAMASTAT integriert und kann dort menügesteuert aufgerufen werden. Die Datenübertragung kann sowohl Originaldaten betreffen als auch Resultate von vorher exekutierten Statistikprozeduren, siehe Abbildung 1.

Im vorliegenden Artikel sollen das Zusammenwirken von WAMASTAT und PROC SASICU sowie die dadurch neu eröffneten Möglichkeiten diskutiert werden.

2. Ablauf des Aufrufes von SASICU aus WAMASTAT

2.1 Interaktive Graphik mit Originaldaten

Nach dem Einstieg ins WAMASTAT gelangt man in gewohnter Weise über den Schirm zur Dateiauswahl in die »Funktionsauswahl«. Hier besteht nun die Möglichkeit, die Originaldaten in die ICU zu transferieren (Funktion »Interaktive Graphik (ICU)«).

Im ersten Subpanel dieser Funktion verlangt WAMASTAT die Auswahl jener Variablen des bearbeiteten Datensets, die auf der horizontalen Achse (x-Achse) dargestellt werden soll, siehe Abbildung 2. Es kann maximal eine Variable selektiert

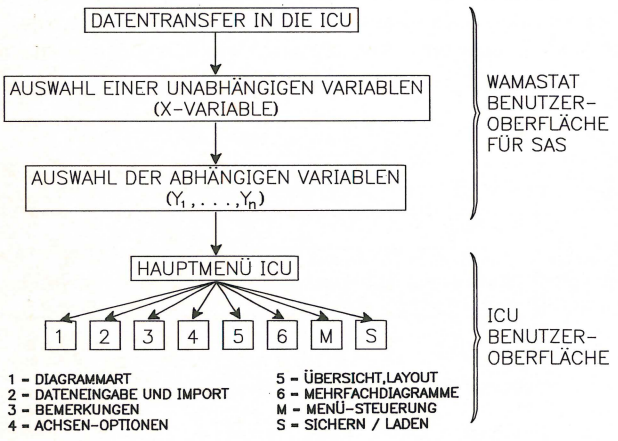

Abb. 2. Ablaufschema für den direkten, interaktiven Datentransfer in die ICU. Der dargestellte Ablauf zeigt jene Einzelschritte, die bei Aufruf des »Direkten Datentransfers in die ICU« (siehe Abb. 1) durchlaufen werden. Innerhalb der Benutzeroberfläche des WAMASTAT werden die X-Variable sowie bis zu zehn Y-Variable menügesteuert selektiert. Dementsprechend werden anschließend die Daten in die ICU übertragen und diese mit ihrem Hauptmenü aufgerufen. Alle weiteren Schritte verlaufen nun auf der Benutzeroberfläche der ICU (siehe die 8 Hauptoptionen am unteren Rand der Darstellung). Nach Verlassen der ICU kehrt der Benutzer zurück zur Ebene des WAMASTAT

werden, der Typ kann jedoch numerisch oder alphanumerisch sein. Für numerische Variable werden die Werte 1:1 übertragen. Wird eine Textvariable für die x-Achse gewählt, ordnet PROC SASICU die Nummer der Beobachtung als numerischen Wert zu (dieser wird von der ICU in jedem Falle verlangt), übergibt jedoch zusätzlich den Inhalt der Textvariablen als X-Label an die ICU. Dadurch erscheint auf der horizontalen Achse in der ICU-Darstellung der alphanumerische Inhalt als »Wert der unabhängigen Variablen«.

Am folgenden Panel werden nur mehr die verbleibenden numerischen Variablen gelistet, aus denen der Benutzer die gewünschten abhängigen Variablen (Y1 bis Yn) auswählt (GDDM – ICU und daher auch SASICU akzeptiert für abhängige Variable nur den numerischen Typ). Durch das WAMASTAT-Panel wird sichergestellt, daß der Benutzer nicht versehentlich eine Textvariable als abhängige Größe darzustellen versucht. Die Anzahl der abhängigen Variablen ist auf 10 beschränkt.

Nach beendeter Variablenauswahl wird die Übertragung nach ICU exekutiert, und der Benutzer gelangt direkt in das Hauptmenü der ICU. In den ICU-Panels zur Dateneingabe und Manipulation erscheinen jedoch die Daten aus der im WAMASTAT gewählten SAS-Datei. Anschließend stehen alle durch die ICU unterstützten Möglichkeiten der interaktiven graphischen Gestaltung offen (siehe auch Abb. 2).

Neben den Optionen 1, 3, 4, 5, 6 und M zur interaktiven graphischen Manipulation sind noch die Datenmanipulation (Option 2) sowie das Sichern/Laden (Option S) von besonderem Interesse. Nach dem Datentransfer kann der Benutzer etwa in das ICU-Panel 2.2 verzweigen. Dort findet er die übertragenen Daten vor und kann sie in der gleichen Weise bearbeiten, als wären sie von Hand eingegeben worden:
– Ausschließen von Variablen (bzw. einzelnen Werten, Ausreißer) aus der graphischen Darstellung
– Skalierung von Variablen relativ zu anderen, entweder punktweise für jeden Wert von X oder gegenüber einem Referenzwert $Y_n(x_i)$
– Transponieren der Datenmatrix
– Sortieren, Verschieben von Datengruppen, etc.
– Regressionsgerade, inkl. der Darstellung mehrerer Regressionsgeraden in einer Graphik

Die genannten Möglichkeiten sind insbesondere deshalb von Interesse, weil weder im SAS noch im WAMASTAT bisher die Möglichkeit bestand, interaktiv ein graphisches Datenscreening zu betreiben. Darüber hinaus besteht auch die Möglichkeit, sowohl Daten als auch das Darstellungsformat (d. h. Diagrammart, Farben, weitere Options) im ICU-internen Format abzuspeichern und wieder zu laden (Option S). Der Benutzer kann sich eine Reihe von Standardformaten, die seiner Problemstellung und seinem Geschmack entsprechen, einmalig herstellen und sodann jeweils nach dem Datentransfer durch SASICU seine »Privatformate« über das Defaultformat »heraufladen«. Diese Vorgangsweise erlaubt eine extrem effiziente graphische Aufbereitung der jeweils neuesten Ergebnisse.

2.2 Interaktive Graphik von statistischen Ergebnissen

SAS bietet die Möglichkeit, Ergebnisse von statistischen Prozeduren (z. B. die in PROC MEANS berechneten Mittelwerte) auf reguläre SAS-Datensets auszugeben. Anläßlich der Integration von SASICU wurde nun für mehrere von WAMASTAT unterstützte Auswertungsprozeduren auch die Ausgabe auf SAS-Datensets und die Übertragung nach ICU installiert. Somit ist es möglich, nicht nur Originaldaten (siehe

```
VARIABLENNAMEN:          X  Y  A    S
                         ------------
                         1  3  1    AB
                         2  4  1    AD
                         3  5  1    AE
                         4  6  2    AF
                         .  7  2    AG
                         8  9  2    AH
                         9  8  3    BA
                        10  5  3    BB
                        12  3  3    BC
                        14  6  3    BD
                        15  2  3    BE

                    * * *  WAMASTAT  * * *

WAMADEMO                                                  27/01/1988
                                                             14:30

Datei : ICU      -
Funktion : Interaktive Graphik (ADMCHART)

        ===> 3.  Y - VARIABLE auswählen          : * 4      *   <====

        Nr    Name        Variablenbeschreibung        Als:  Typ Stellen
        ------------------------------------------------------------------
        0001  S                                        X001   T     02
        0002  X                                        Y001   Z     08
        0003  Y                                        Y002   Z     08
  >>>>  0004  A                                              Z     08

                                                        Seite 001 von 001
1-EXEC     4-Letzte Auswahl Rücksetzen                 6-Gewählte Variable
2-Info        8-STORNO      3/9-FUNKTIONSAUSWAHL      10-Vor        11-Rück

                Data Group Names -------> X          Y          A
                Data Group (Z) Values --> 1          2          3

              *** X Values     X Labels     Y1         Y2         Y3
              001 1            AB           1          3          1
              002 2            AD           2          4          1
              003 3            AE           3          5          1
              004 4            AF           4          6          2
              005 5            AG           .          7          2
              006 6            AH           8          9          2
              007 7            BA           9          8          3
              008 8            BB           10         5          3
              009 9            BC           12         3          3
              010 10           BD           14         6          3
              011 11           BE           15         2          3
              X   .                         .          .          .
Commands: D (Delete) R (Repeat) FIT (Least Squares Fit) S (Select) X (Exclude
          / (Scroll Here) M (Move) A (After) B (Before) I (Insert)
          See Help for More

PF: 1=Help 2=Save/Load 3=End 4=Print 5=Display 7=Up 8=Down 10=Left 11=Right
    12=Home
```

Abb. 3. Datenformat und Datenzugriff auf verschiedenen Benutzerebenen während des Transfers in die ICU. Im oberen Teil sind die Originaldaten (als Zeilen und Spalten) dargestellt. In der Mitte sind Teile des WAMASTAT-Menüs gezeigt, das bei der Variablenauswahl durchlaufen wird. Der untere Teil der Abbildung zeigt das ICU-Menü 2.2 zur Datenmodifikation innerhalb der ICU nach durchgeführtem Transfer. Hier können die übertragenen Daten nochmals modifiziert werden, ehe man sie mit PF5 (siehe Optionsliste am unteren Rand des Menüs) zur Anzeige bringt (vgl. Abb. 4). Man beachte, daß die Textvariable S im WAMASTAT-Menü als X-Variable ausgewählt wurde und daher ihr Inhalt in der ICU als X-Labels aufscheint

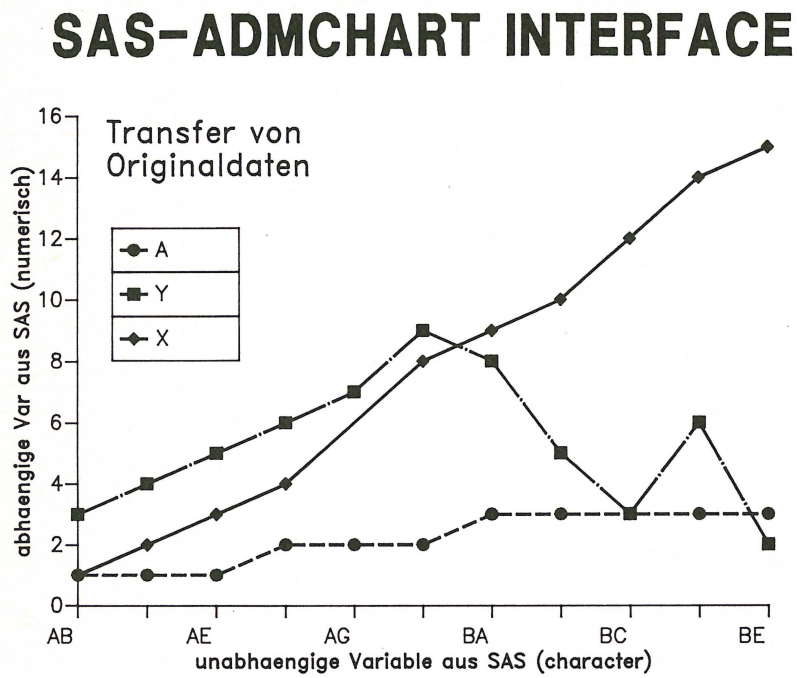

Abb. 4. Beispiel für einen direkten Datentransfer in die ICU. Aus einer WAMASTAT-Datei mit der in Abbildung 3 gezeigten Struktur werden interaktiv die gewünschten Variablen selektiert, automatisch in die ICU übertragen und dargestellt. Die Achsenbeschriftungen, der Titel sowie die Bemerkung »Transfer von Originaldaten« wurden interaktiv in der ICU hinzugefügt

Abschnitt 2.1), sondern auch vorverrechnete Werte der interaktiven Graphik zuzuführen (Abb. 1). Wesentlich dabei ist, daß für jede Art von Auswertung eine spezielle graphische Darstellungsform als Standardoption (Default) im WAMASTAT festgesetzt wurde. So werden etwa die Häufigkeiten in einzelnen Zellen eines statistischen Modells über die SAS-Prozedur »PROC FREQ« (von WAMASTAT unterstützt) berechnet und dann nach ICU übertragen; die ICU wird dabei automatisch mit dem passenden Format (Turmdiagramm) initialisiert.

3. Beispiele

3.1 Übertragung von Originaldaten aus WAMASTAT

Abbildung 3 zeigt die Daten einer in WAMASTAT erstellten Testdatei sowie den zugehörigen Auswahlschirm für die zu transferierenden Variablen. Als unabhängige Variable wurde die Textgröße S gewählt, die abhängigen Variablen X, Y und A sind numerische Größen. Nach beendigter Auswahl werden die Daten automatisch in die ICU transferiert, und der Benutzer gelangt in das ICU-Hauptmenü. Um sich vom korrekten Transfer zu überzeugen, kann man in das Panel 2.2 zur Datenmanipulation innerhalb der ICU verzweigen. Dort erscheinen die Daten so, als wären sie direkt über das ICU-Panel eingegeben worden. Man beachte, daß der Inhalt der für die »X-Achse« gewählten Textvariablen S als »X-Label« erscheint. Die in der ICU unbedingt erforderlichen Werte für die unabhängige Variable werden durch das Interface generiert. Ebenso werden die Namen der abhängigen SAS-Variablen als »DATA GROUP NAMES« in die ICU übertragen, siehe Abbildung 3. Fehlende Werte (z. B. der 5. Wert der abhängigen Variablen X) werden als solche übertragen. Mit der Taste PF5 wird die Graphik schließlich angezeigt und steht zur interaktiven Bearbeitung zur Verfügung (Abb. 4).

Erwähnenswert ist noch, daß übertragene Originaldaten mit den in der ICU vorgesehenen Optionen nur zum Zwecke der graphischen Darstellung modifiziert bzw. verrechnet werden können. Von großem praktischem Nutzen sind insbesondere Möglichkeiten der Dateneingabe, Modifikation und Interpretation, welche bereits in Abschnitt 2.1 besprochen wurden.

3.2 Übertragung von Auswertungsergebnissen aus WAMASTAT

Für alle in Abbildung 1 gelisteten statistischen Verfahren kann die Übertragung der Ergebnisse in die ICU angefordert werden.

Sämtliche Möglichkeiten der Modifikation innerhalb der ICU stehen dann in gleicher Weise wie nach der Übertragung von Originaldaten offen. Als Beispiel zeigt Abbildung 5 die Darstellung von Häufigkeiten über zwei Variablen. Während der Datenübertragung wird die ICU mit dem passenden Format (Turmdiagramm, entsprechende Achsenbeschriftung) initialisiert. Der Benutzer kann dann beliebige Bemerkungen beifügen (siehe Abb. 4, »Transfer von Originaldaten«) bzw. Farben, Überschrift oder Legenden interaktiv ändern.

4. Diskussion

Wesentliches Merkmal der beschriebenen Installation ist ihre volle Kompatibilität mit SAS. Einerseits kann jedes speziell erstellte SAS-Programm auf WAMASTAT-Dateien zugreifen, andererseits können im SAS erstellte Dateien sofort von WAMASTAT angesprochen werden. Entscheidet sich daher ein Kliniker zur Benutzung des WAMASTAT, muß er nicht (wie bei vielen Auswertesystemen auf PC-Basis) fürchten, daß alle Daten in ein anderes Programmsystem (oder gar auf einen anderen Computer) übertragen werden müssen, sollte das zu Beginn gewählte System (d. h. WAMASTAT) eine gewünschte Auswertung nicht im Menü vorgesehen haben. WAMASTAT ist »nach oben offen«, die einzige Beschränkung ist die (allerdings extrem hohe) Leistungsfähigkeit von SAS. Andererseits ist die Prozedur SASICU nach den Richtli-

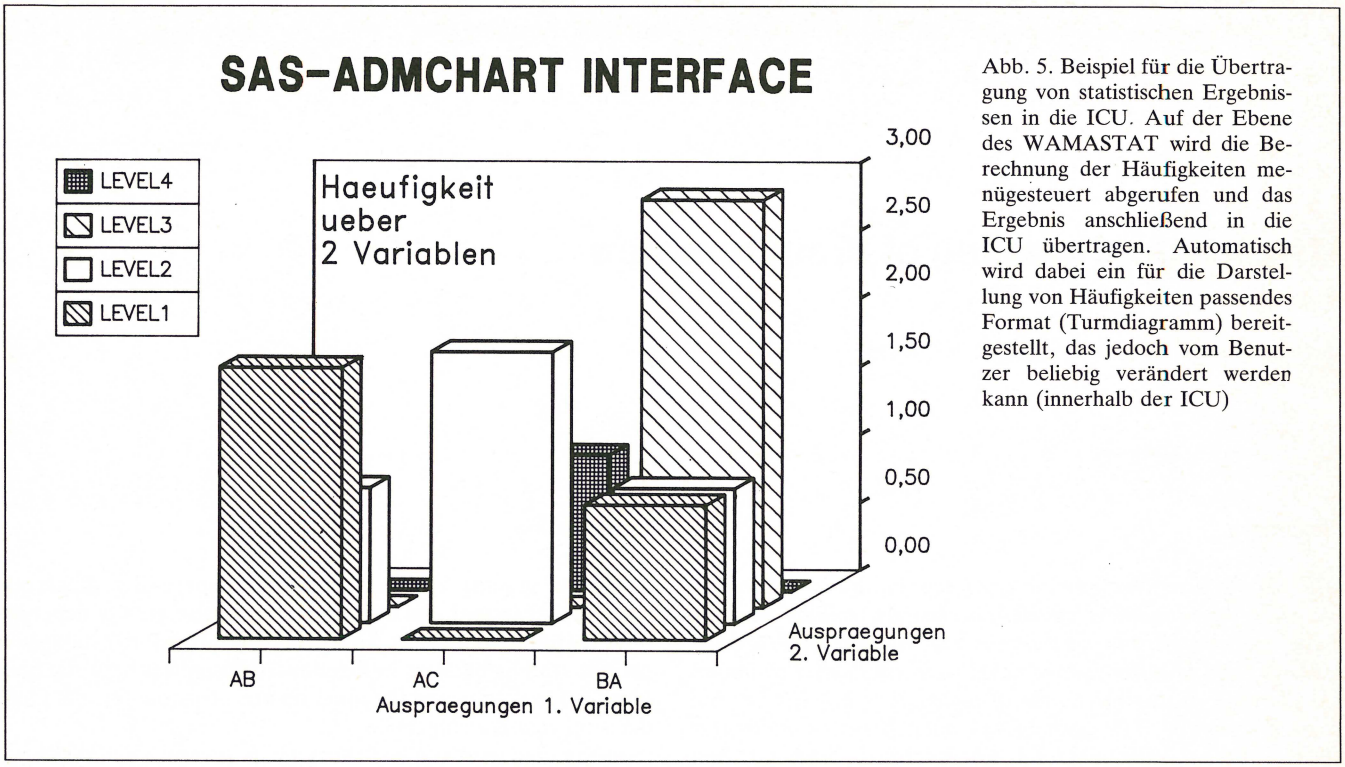

Abb. 5. Beispiel für die Übertragung von statistischen Ergebnissen in die ICU. Auf der Ebene des WAMASTAT wird die Berechnung der Häufigkeiten menügesteuert abgerufen und das Ergebnis anschließend in die ICU übertragen. Automatisch wird dabei ein für die Darstellung von Häufigkeiten passendes Format (Turmdiagramm) bereitgestellt, das jedoch vom Benutzer beliebig verändert werden kann (innerhalb der ICU)

nien für die Erstellung benutzerdefinierter SAS-Prozeduren verfaßt und gewährt demgemäß volle Kompatibilität mit SAS (auch in kommenden Versionen).

Auch der zweite Teil von SASICU, nämlich die Aufrufe der GDDM-Routinen aus einem PL/1-Programm, ist streng nach den Richtlinien für GDDM-Programmierung erstellt, so daß auch hier mit voller Aufwärtskompatibilität gerechnet werden kann.

Schließlich steht es dem Benutzer auch offen, SASICU direkt in einem selbsterstellten SAS-Programm aufzurufen, etwa um die Ergebnisse einer Auswertung darzustellen, die nicht über das Menüsystem des WAMASTAT angeboten wird. Somit ist auch für die interaktive Graphik in speziell erstellten SAS-Programmen volle Kompatibilität gegeben. Diese Anwendung kommt in Frage, wenn etwa »private Prozeduren« in WAMASTAT durch EDV-Techniker installiert werden, anschließend jedoch von Klinikern verwendet werden sollen, für die der Komfort einer interaktiven graphischen Aufbereitung als Standard gelten kann.

Danksagung

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Histological grading of brain tumours

J. R. Iglesias, C. Aruffo, J. Esparza, E. Kazner

Summary

Ten histological characteristics (diffuse infiltration, necrosis, vascular abnormalities, vascular occlusions, cellular and nuclear polymorphism, pericaryon size, typical and atypical mitoses, and undifferentiated cells) were considered as important in determining the Grade of malignancy in 1462 nervous system tumours. The manner in which these characteristics change from Grade to Grade was analysed. Some of these characteristics change significantly between Grades II and III: necrosis, vascular abnormalities, vascular occlusions and typical mitoses. Diffuse infiltration, cellular polymorphism and pericaryon size, on the other hand, change importantly between Grades I and II. The presence of the remaining characteristics (nuclear polymorphism, undifferentiated cells and atypical mitoses) changes from one Grade to the other. The combination of the characteristics present and their intensity has allowed us to obtain a precise and objective grading in the 175 tumours of our testing field. This analysis was done with the help of a personal computer.

Zusammenfassung

Für die Bestimmung des Malignitätsgrades in 1462 Tumoren des Nervensystems wurden zehn histologische Merkmale (diffuse Infiltration, Nekrose, Gefäßanomalien, Thromben, Zell- und Kernpolymorphie, Größe des Zellkörpers, typische und atypische Mitosen, undifferenzierte Zellen) berücksichtigt. Die Variation der Merkmale zwischen jedem Malignitätsgrad wurde untersucht. Einige dieser Merkmale verändern sich deutlich beim Wechsel von Grad II zu Grad III: Nekrose, Gefäßanomalien, Thromben und typische Mitosen. Währenddessen verändern sich zwischen Grad I und II deutlich die Merkmale diffuse Infiltration, Zellpolymorphie und Größe des Zellkörpers. Die übrigen Merkmale (Kernpolymorphie, undifferenzierte Zellen und atypische Mitosen) verändern sich von einem Grad zum anderen. Das Muster der vorhandenen Merkmale und ihr Ausprägungsgrad erlaubten uns ein exaktes und objektives Bestimmen des Malignitätsgrades in diesen 175 Tumoren unserer Testgruppe. Diese Untersuchung wurde mit Hilfe des Bayeschen Systems auf einem PC durchgeführt.

Introduction

Tumoural grading is a very important aspect of a diagnosis since the treatment and outcome of each case greatly depends on it (MØRK et al., 1986). However, it is difficult to establish a precise grading because well delimited boundries between one Grade of malignity and the other do not exist and thus the final decision remains subjective.

In the course of the last thirty years several attempts have been made to establish an adequate system of grading. The first grading scale for tumours of the nervous system was developed by KERNOHAN et al. (1949). They divided astrocytomas in four degrees of malignity. Later RINGERTZ (1950) introduced a grading scale of three degrees for astrocytomas, ependymomas and oligodendrogliomas. A statistical analysis of the grading of brain tumours was introduced by SCHRODER et al. (1968a, 1968b, 1970). The morphological criteria for a grading were given by GULOTTA (1981) and by ZÜLCH (1980, 1981). In general terms, it is accepted (ZÜLCH, 1979) that the criteria which determine malignity are: the number of cells, cellular and nuclear polymorphism, the presence of typical and atypical mitoses, vascular proliferation, necrosis and tumoural infiltration.

These features, considered to indicate malignity, combine in numerous manners. Therefore, it is frequent to have cases in which it is difficult to decide which is the degree of malignity. We wish to present a computerized method for the grading of brain tumours that can offer greater objectivity and thus could lead to a unification of criteria. This method has also allowed us to analyse in detail which characteristics change and how they change from one degree of malignity to the other.

Materials and Methods

The 1462 nervous system tumours studied were fixed in 10 % formaldehyde. Different areas (1 to 10 samples) of the tumours were included in paraffin. The following stainings were made: hematoxylin and eosin, cresyl violet, and a trichromic staining. All samples of each tumour were studied and the existence or absence of 50 previously selected histological characteristics was noted (IGLESIAS et al., 1986b). When an histological characteristic was present the observer indicated its degree: low, middle or high (+, ++, +++).

1287 tumours were used as a data base. The grading used in our data base was based on that given by ZÜLCH (1981). The tumours studied were distributed as follows:

Table 1. Presence of characteristics indicating malignity in 1287 nervous system tumours given in %

Characteristic	Grade I	II	III	IV
Diffuse infiltration	36.48	87.81	89.62	81.91
Necrosis	22.16	24.63	71.69	85.09
Vascular abnormalities	64.86	68.66	84.90	92.66
Vascular occlusions	11.35	12.19	51.89	64.06
Nuclear polymorphism	70.27	82.58	97.17	96.82
Cellular polymorphism	36.21	70.64	80.19	83.37
Pericaryon size	49.46	86.57	89.62	88.75
Typical mitoses	12.16	10.95	72.64	85.33
Atypical mitoses	0.54	2.99	55.66	73.35
Undifferentiated cells	41.35	45.02	65.10	94.37

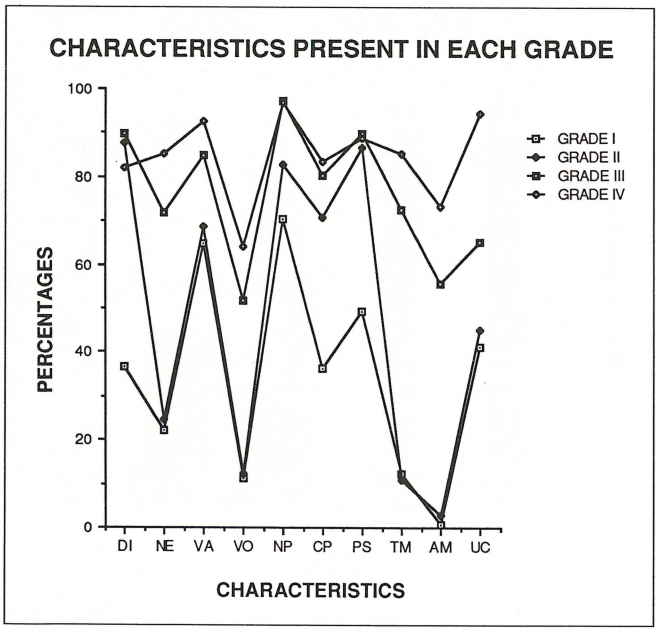
Grade I: 370 Tumours
- Meningiomas: endotheliomatous, fibrous, and transitional
- Pilocytic astrocytoma
- Hypophysis adenoma
- Ependymoma and Subependymoma

Grade II: 402 Tumours
- Astrocytoma: fibrillary, protoplasmatic, and gemistocytic
- Oligodendroglioma and mixed oligoastrocytoma

Grade III: 106 Tumours
- Anaplastic astrocytoma
- Anaplastic oligodendroglioma

Grade IV: 409 Tumours
- Meningosarcoma
- Glioblastoma and gliosarcoma
- Medulloblastoma
- Neuroblastoma

Fig. 1. Graph depicting the distribution of the ten histological characteristics studied considered to be indicative for the degree fo malignity of a tumour. DI-diffuse infiltration; NE-necrosis; VA-vascular abnormalities; VO-vascular occlusions; NP-nuclear polymorphism; CP-cellular polymorphism; PS-pericaryon size; TM-typical mitoses; AM-atypical mitoses; UC-undifferentiated cells



All those tumours which corresponded to a given degree were analysed separately.

To decide which of the 50 characteristic we studied is related to malignity the following heuristic criteria were used: the percentage of presence must have a tendency to increase with increasing malignity independent of the final diagnosis. Thus we selected the following characteristics as being those which indicate degree of malignancy: diffuse infiltration, necrosis, vascular abnormalities, vascular occlusions, cellular and nuclear polymorphism, pericaryon size, typical and atypical mitoses, undifferentiated cells. In all cases of our data base we determined the percentage of appearance of each of these ten characteristics and their intensity (low, medium or high).

All our data was analysed with a Bayesian system (IGLESIAS et al., 1983, 1986a, 1986b; PFANNKUCH et al., 1987). The probability a priori for each Grade was assumed to be 0.25. Utilizing the percentages of the ten selected characteristics it is possible to calculate the probability a posteriori for a new tumour to belong to one of the four Grades of malignancy. To validate our method we calculated the grading (probability a posteriori) in the remaining 175 tumours.

All calculations were made with a personal Computer (PC) Commodore/8032 with a dual floppy disk/8050 and a printer/8032p. All programs were written in BASIC. This program was also adapted to a pocket computer Cassio Fx-750p with 4K RAM.

Results

Data base

For the data base the absence or presence of each of the ten characteristics considered to indicate malignity was calculated in percentages for each Grade (Table 1, Fig. 1).

When analysing the data base we found that in the ten characteristics considered as important for the grading of malignancy an increase in the total percentage of each characteristic present is seen with increasing malignity (Table 1, Fig. 1).

For necrosis (NE), vascular occlusions (VO), and typical mitoses (TM) a very drastic change is seen between Grades II and III. These characteristics are seen in less than 25 % of the cases which correspond to a Grade I or II, whereas they are present in over 50 % of the cases corresponding to Grades III and IV (Table 1). A boundry between Grades II and III may also be given by the presence of vascular abnormalities which although present in a relatively high percentage of cases of Grade I and II (65 and 69 %), they increase drastically between grades II and III (69 and 85 % respectively).

The clear cut boundaries between Grades I and II are given, on the other hand, by the following characteristics: diffuse infiltration (DI), cellular polymorphism (CP) and an increase in cellular size (CS). When considering these last three criteria practically no boundaries can be set between Grade II, III and IV. Interestingly the percentage of cases with diffuse infiltration is higher in Grades II and III (88 and 90 %) and decreases slightly in Grade IV (82 %).

Nuclear polymorphism (NP) changes from Grade I (70 %) to II (83 %) and then again from Grade II (83 %) to III (97 %). The amount of undifferentiated cells (UC) also changes in two steps, between Grades II (45 %) and III (65 %) and between Grades III (65 %) and IV (94 %). The presence of atypical mitoses (AM) changes drastically from Grade II (3 %) to Grade III (56 %) and then again from Grade III (56 %) to Grade IV (73 %).

To further determine the utility of each of these characteristics in differentiating one Grade of malignity from the other, the changes in intensity of each characteristic were analysed in each Grade.

Diffuse infiltration of the tumour was absent in 64 % of the cases of Grade I. When present it was very similar for degrees +, ++, and +++ (12, 10 and 18 % respectively). In Grades II, III and IV diffuse infiltration was always very intensely present (Fig. 2).

A very high percentage of tumours of Grade I and II (78 and 75 %) do not have necrosis. Necrosis increases clearly with the degree of malignity. This increase is notorious between Grades II (25 %) and III (72 %) being necrosis predominantly of moderate intensity (Fig. 3).

Fig. 2. Graph depicting the distribution of the characteristic diffuse infiltration (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high

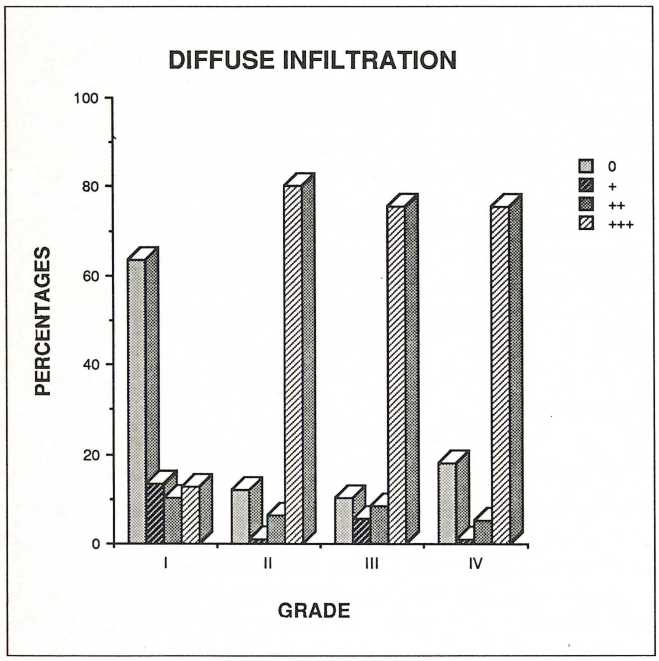


Fig. 3. Graph depicting the distribution of the extent of necrosis (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high

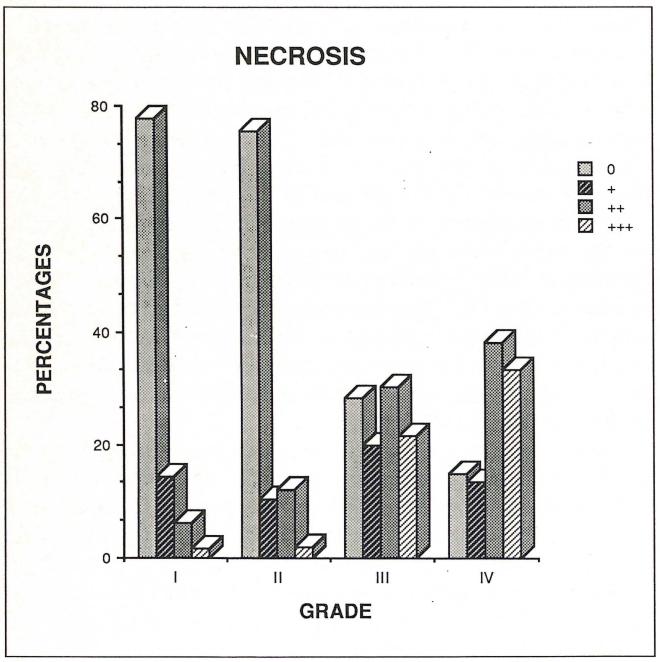


Fig. 4. Graph indicating the distribution of the amount of anomalous vessels (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high

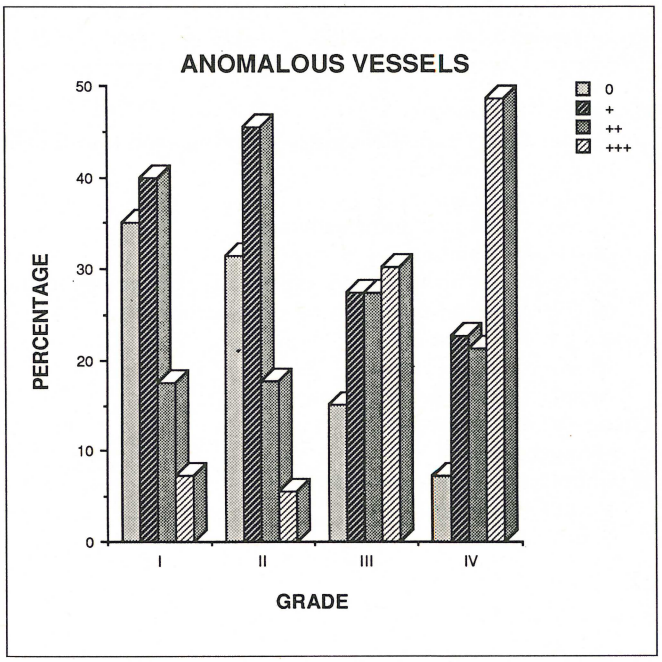
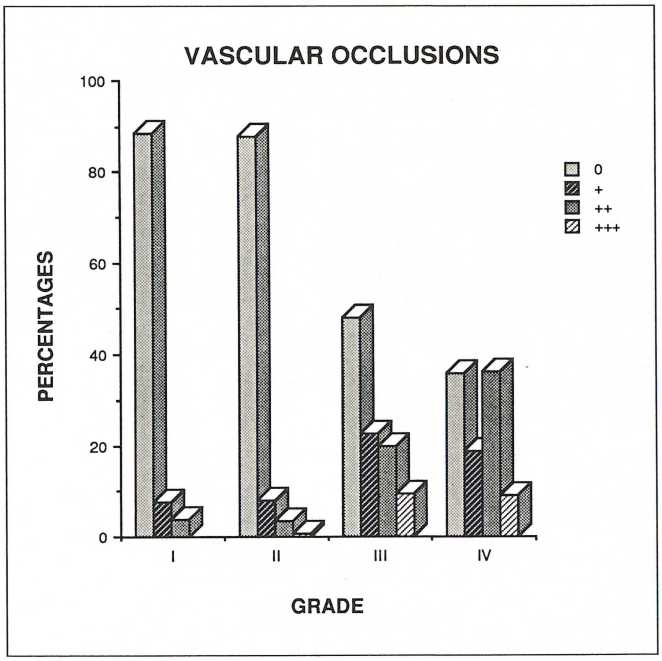


Fig. 5. Graph depicting the distribution of the amount of vascular occlusions (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high



Anomalous vessels are present in a high percentage of tumours even in Grade I (65 %). When present they are found in a low degree (+) except in Grade IV in which the amount of anomalous vessels present is very high (Fig. 4). It is interesting to notice that in tumours of Grade I and II anomalies which are mostly of low intensity correspond to abnormalities in the vessels and in the capillary net, whilst in tumours of Grade III and IV aside from these abnormalities there is an anomalous endothelial proliferation which leads to the formation of glomeruli. This is evident in that the intensity of abnormalities is very high.

Fig. 6. Graph depicting the distribution of the amount of cellular polymorphism (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high

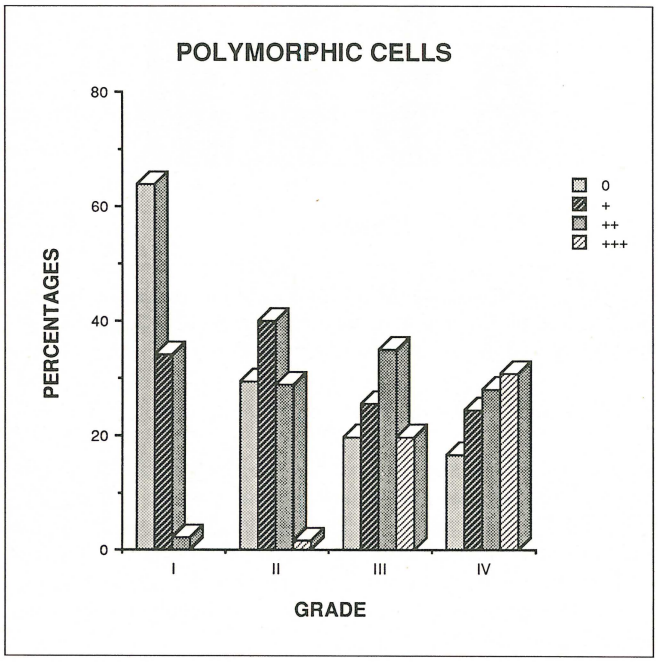
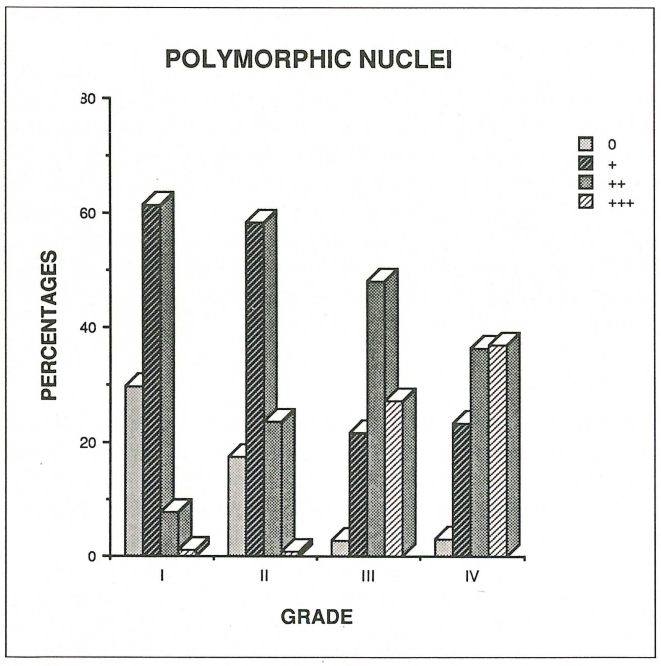


Fig. 7. Graph which shows the distribution of the degree of nuclear polymorphism (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high



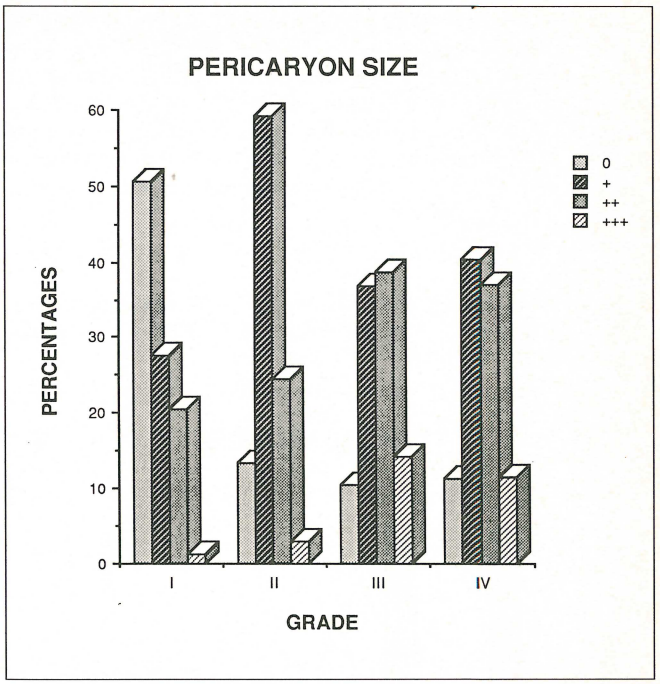


Fig. 8. Graph illustrating the distribution of the amount of cells of different sizes (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high

In malignant tumours (Grade III and IV) between 50 and 65 % of the tumours present vascular occlusions. These are motly of low to middle intensity. In tumours of low malignity trombi are found in approximately 10 % of the cases once again when present then in low (+) intensity (Fig. 5).

Cellular polymorphism is only present in 36 % of Grade I tumours. When present it is in low intensity. With increasing malignity there is an increase in the number of cases which present cellular polymorphism as well as an increase in the intensity of cellular polymorphism (Fig. 6). However, it must be said that even in Grade IV tumours a relatively high percentage of tumours (25 %) have cellular polymorphism of low intensity. The percentage of low malignity (Grades I and II) tumors with polymorphic nuclei is very high (61 and 58 %). However, intensity is very low. In tumours of more malignity (Grade III and IV) nuclear polymorphism increases not only in the amount of cases presenting it but also in intensity. Most of these tumours have a moderate amount of polymorphic nuclei, however, and particularly in Grade IV tumours high intensity is seen very frequently (37 %) (Fig. 7).

The increasing cellular size was indicated by +, ++, +++. In many tumours of the nervous system, however, it is not possible to distinguish clearly the cellular limits and thus we marked this characteristic as being absent. In 50 % of the tumours of Grade I it is not possible to delimit the pericaryon with routine histological stainings. The tumour is seen as an undifferentiated mass in which tumoural nuclei swim. When the pericaryon is celarly delimited the cells are almost always small or middle sized. With increasing malignity cellular pericaria are distinguished much better and although small and medium sized cells predominate big cells are also seen (Fig. 8).

Few typical mitoses are seen in tumours of Grade I (12 %) and II (11 %). A very notorious increase in the total amount of typical mitoses is seen between Grade II (11 %) and III (73 %). With increasing malignity there is not only an increase in the number of cases presenting typical mitoses but also an increase in the intensity. In such a manner that in Grade I tumours only 12 % of the cases studied presented typical mitoses (+ = 9 % and ++ = 3 %) whereas in Grade IV tumours 85 % of the cases had typical mitoses (+ = 20 %, ++ = 28 %, +++ = 37 %). The important difference in the intensity of typical mitoses seen between Grade II (which is very similar to Grade I) and Grade III (which is very similar to Grade IV) permits a clear delimitation between these two malignity groups (Fig. 9).

Fig. 9. Graph which shows the distribution of the amount of typical mytoses (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high

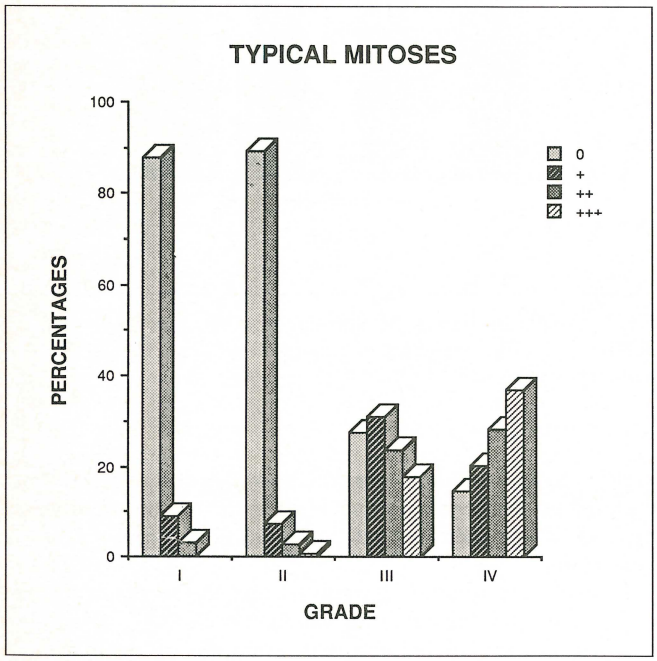
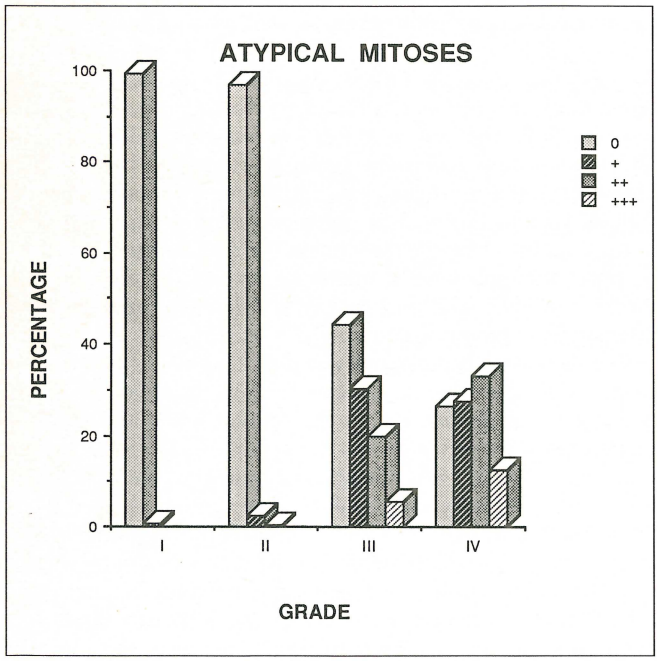


Fig. 10. Graph depicting the distribution of the amount of cells with atypical mytoses (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high



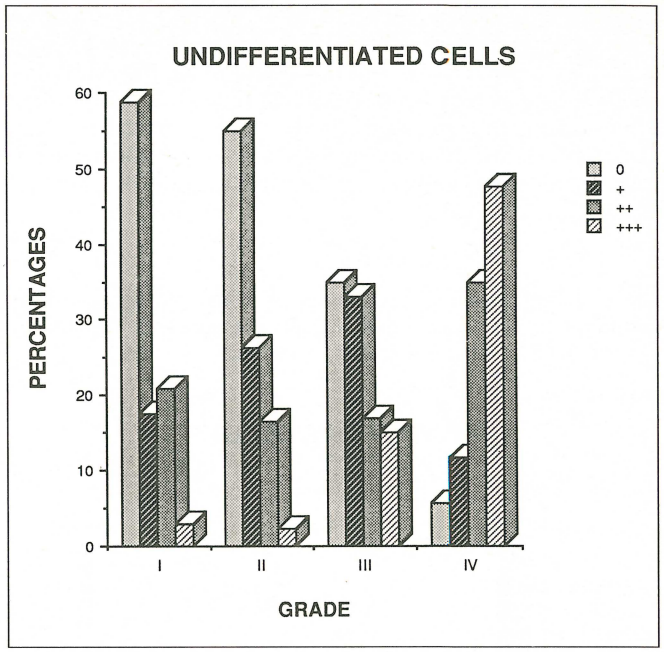


Fig. 11. Graph illustrating the distribution of the amount of undifferentiated cells (in %) present in tumours of grades I, II, III, and IV. O-not present, +-low, ++-middle, +++-high

Atypical mitoses are almost never present in Grade I (0,5 %) and II (3 %) tumours. Many tumours of Grade III and IV have atypical mitoses (56 and 73 % respectively). In these cases a low to moderate intensity predominates (Fig. 10). The lack of atypical mitoses in Grades I and II can be of great help to delimit these low malignity tumours from high malignity tumours Grades III and IV.

Although the amount of undifferentiated cells augments with increasing malignity it is possible to see a high percentage of undifferentiated cells in Grade I tumours (41 %). The intensity of undifferentiated cells in Grades I and II is low to moderate. In Grade III tumours there is a notizable increase in the total number of cases presenting undifferentiated cells (65 %). In these cases the intensity is predominantly low (33 %). In Grade IV tumours almost all cases have undifferentiated cells (94 %). Their intensity is moderate to high (35 % and 48 % respectively) (Fig. 11).

Testing field

When the computer determined the degree of malignity based on the data concerning the ten characteristics considered we obtained a correct grading in the first instance in 84 % of the cases. When we considered both first and second gradings as correct we obtained an accuracy in 99 % of the cases (Table 2). Only one case was incorrectly Graded in the first and second posibilities (Table 3). In this case we were dealing with a medulloblastoma which had all signs of malignity but a total abscence of atypical mitoses and only very few typical mitoses.

Table 2. Testing of the grading of 175 tumours of the nervous system based on the discriminant analysis of 1287 cases (percentages are given in parenthesis)

Neuropathological grading	Number of tumours	1st grading	2nd grading
Grade I			
Angioma	10	9 (90)	1 (10)
Ependymoma	5	5 (100)	
Haemangioblastoma	6	5 (84)	1 (16)
Hypophysis adenoma	19	19 (100)	
Meningioma	32	31 (97)	1 (3)
Neurofibroma	9	8 (89)	1 (11)
Pilocytic Astrocytoma	1	1 (100)	
Subependimoma	1	1 (100)	
Total	83	79 (95)	4 (5)
Grade II			
Astrocytoma	14	10 (71)	4 (29)
Oligoastrocytoma	12	9 (75)	3 (25)
Oligodendroglioma	7	4 (57)	3 (43)
Total	33	23 (70)	10 (30)
Grade III			
Anaplastic astrocytoma	7	3 (43)	4 (57)
Anaplastic oligodendroglioma	7	4 (57)	3 (43)
Total	14	7 (50)	7 (50)
Grade IV			
Glioblastoma	20	20 (100)	
Gliosarcoma	1	1 (100)	
Medulloblastoma	2	1 (50)	
Meningosarcoma	1	1 (100)	
Metastasis	20	14 (70)	6 (30)
Neuroblastoma	1	1 (100)	
Total	45	38 (84)	6 (13)
Total	175	147 (84)	27 (15)

Discussion

With mathematical methods we have been able to determine that brain tumours can be divided into four Grades when considering exclusively their histological characteristics, since they change from one Grade to another in a very determined manner. These findings would confirm the classification of ZÜLCH (1981) and that of SMITH et al. for oligodendrogliomas (1983) in which tumours are also graded in four groups. Our mathematical analysis indicates, thus, that the grading of RINGERTZ (1950) and HENSCHENS (1955) are probably simplified since it is evident from our analysis that a palpable difference can be established between Grades I to IV.

Various authors (KAZNER et al., 1981) believe that histological Grades are only significant when they are used to classify tumours of one same group. In this study we have been able to demonstrate that, because the characteristics indicating malignity are constant in all tumour types, grading is significant when studying any type of tumour and can be comparable. It is important, however, to distinguish, when talking about prognosis, between the histological grading and the significance of the grading for the prognosis, since prognosis also depends on the localization of the tumour, treatment, risk factors individual to each patient, etc. Thus a Grade I meningioma can not have the same prognosis as a Grade I hypophysis adenoma, although histologically they have the same degree of malignity. This difference in prognosis is given by the different localization and by the role which hormones may play. This example may be applied to many other tumours of the nervous system.

From the analysis of each of the histological characteristics which determine malignity it is evident that their increase is not always linear or directly proportional to the Grade but in most cases it »jumps«. Such »jumps« are more evident between Grade II and III for characteristics such as necrosis, vascular abnormalities, vascular occlusions, typical and atypical mitoses and undifferentiated cells and between Grades I and II for diffuse infiltration, and cellular polymorphism. A detailed analysis of these changes permits an easy and objective differentiation of tumours Grades I, II, and III. To differentiate Grades III from IV it is necessary to analyse the intensity of each characteristic. Thus to distinguish Grades III and IV it is not so much the presence or absence of a characteristic which is important but rather the intensity of that characteristic, for example polymorphic nuclei and typical mytoses which are present in higher intensity in Grade IV as in Grade III.

This method reflects the same problems with which the pathologist is faced when giving a grading. There are characteristics which speak in favour of a low malignity whilst others in the same tumour speak for high malignity. The greater difficulty in establishing grading was seen in those tumours which lay in the limit between one Grade and the immediately neighbouring one. The advantage of this system is that each characteristic will be analyzed in a more objective manner and their combination (1024 possible combinations when considering presence or absence of each of the ten characteristics) is better and more rapidly analyzed with a computer. With this method the importance of each single characteristic can be analyzed separately.

The utilization of ten histologic characteristics provides a system which can be easily applied to every patient and eventually could allow the establishment of a more precise outcome prognosis for each patient (MØRK et al., 1986).

A differential grading expressed in percentages of probabilities a posteriori is provided with this method. This expresses the fact that a Grade is not a static classification but rather a continuous event. Therefore, we have considered that when we have two continuous Grades both the first and second suggested diagnoses should be considered as correct. Although a precise histological Grade can be obtained with the help of a computer the final Grade must be decided by the

Table 3. Example of how grading probabilities were calculated (in %)

Tumour 74	Anaplastic Astrocytoma Grade III	
	Computer Grading: Grade IV	60.27
	Grade III	39.27
Tumour 83	Fibrillary Astrocytoma Grade II	
	Computer Grading: Grade I	75.59
	Grade II	24.08
Tumour 175	Medulloblastoma Grade IV	
	Computer Grading: Grade III	53.96
	Grade II	19.10
	Grade IV	18.00
	Grade I	8.93

handling physician, who will evaluate the histological criteria, location, patients condition and other factors which can influence the outcome of the patient.

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Address correspondence to: The authors' adresses: Dr. J. R. Iglesias, Neurochirurgische Klinik, Universitätsklinikum Charlottenburg und Rudolf-Virchow-Krankenhaus der FU Berlin, Augustenburger Platz 1, D-1000 Berlin 65, FRG; C. Aruffo, Institut für Neuropathologie, Universitätsklinik Steglitz, Freie Universität Berlin, Hindenburgdamm 30, D-1000 Berlin 45, FRG

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Ein Schätzer für den Intraklass-Korrelationskoeffizienten (IKK) im einfachen Klassifikationsmodell und dessen approximative Varianz

E. Stavrakakis

Zusammenfassung

Der Intraklass-Korrelationskoeffizient spielt in der Tierzüchtung (und in der Genetik im allgemeinen) eine große Rolle. In der vorliegenden Arbeit wird ein neuer Schätzer $\tilde{\varrho}$ dieses Koeffizienten präsentiert, der allem Anschein nach besser ist als $\hat{\varrho}$. Die approximative Varianz von $\tilde{\varrho}$ wird ebenfalls geschätzt. Beide Schätzer sind Funktionen von $\tilde{\vartheta}$, der ein besserer Schätzer von $\vartheta = \sigma_\alpha^2/\sigma_e^2$ ist als der übliche $\hat{\vartheta}$.

Summary

The intraclass correlation coefficient plays an important role in the animal breeding (and in genetics generally). A new estimator $\tilde{\varrho}$ of this coefficient is presented which seems to be better than the usual $\hat{\varrho}$. The approximate variance of $\tilde{\varrho}$ is estimated. Both estimators are functions of $\tilde{\vartheta}$ which is a better estimator of $\vartheta = \sigma_\alpha^2/\sigma_e^2$ than the usual $\hat{\vartheta}$.

1. Einleitung

Die Modellgleichung bei einfacher Klassifikation mit zufälligen Effekten lautet:

$$y_{ij} = \mu + \alpha_i + e_{ij} \qquad (1)$$
$$i = 1, \ldots, r;\ j = 1, \ldots, n_i$$

$\alpha_1, \ldots, \alpha_r$ ist eine Stichprobe von unabhängigen, nicht beobachtbaren Zufallsvariablen mit

$$\alpha_i \sim N(0, \sigma_\alpha^2),\ i = 1, \ldots, r.$$

$\{e_{ij},\ i = 1, \ldots, r;\ j = 1, \ldots, n_i\}$ ist ebenfalls eine Stichprobe von unabhängigen, nicht beobachtbaren Zufallsvariablen mit $e_{ij} \sim N(0, \sigma_e^2)$. Beide Stichproben sind unabhängig.

Der Intraklass-Korrelationskoeffizient oder Innerklassenkorrelationskoeffizient wird für das obige Modell durch folgende Beziehung definiert:

$$\varrho = \sigma_\alpha^2/(\sigma_\alpha^2 + \sigma_e^2). \qquad (2)$$

Folgende Schreibweise (Formel) wird im weiteren verwendet:

$$\varrho = \vartheta/(1 + \vartheta) \text{ mit } \vartheta = \sigma_\alpha^2/\sigma_e^2. \qquad (3)$$

Die Größe ϱ spielt in der Tierzüchtung (und in der Genetik im allgemeinen) eine große Rolle.

Der übliche Schätzer $\hat{\varrho}$ für ϱ ergibt sich aus dem Schätzer

$$\hat{\vartheta} = \hat{\sigma}_\alpha^2/\hat{\sigma}_e^2, \text{ wobei} \qquad (4)$$
$$\hat{\sigma}_\alpha^2 = (MSA - MSE)/\lambda,\ \hat{\sigma}_e^2 = MSE \qquad (5)$$

$$\text{und } \lambda = \frac{1}{r-1}\left(N - \frac{\sum_{i=1}^{r} n_i^2}{N}\right),\ N = \sum_{i=1}^{r} n_i \qquad (6)$$

MSA und MSE sind die üblichen Mittelquadratsummen der einfachen Varianzanalyse und folgendermaßen definiert:

$$MSA = \frac{1}{r-1}\sum_{i=1}^{r} n_i\,(\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot})^2 = \frac{1}{r-1}\left(\sum_{i=1}^{r} n_i \bar{y}_{i\cdot}^2 - N\bar{y}_{\cdot\cdot}^2\right)$$

$$MSE = \frac{1}{N-r}\sum_{i=1}^{r}\sum_{j=1}^{n_i}(y_{ij} - \bar{y}_{i\cdot})^2 \qquad (7)$$
$$= \frac{1}{N-r}\left(\sum_{i=1}^{r}\sum_{j=1}^{n_i} y_{ij}^2 - \sum_{i=1}^{r} n_i \bar{y}_{i\cdot}^2\right).$$

Für $\hat{\varrho}$ gilt also:

$$\hat{\varrho} = \hat{\vartheta}/(1 + \hat{\vartheta}) = \hat{\sigma}_\alpha^2/(\hat{\sigma}_\alpha^2 + \hat{\sigma}_e^2). \qquad (8)$$

Man kann leicht feststellen, daß

$$E(\hat{\sigma}_\alpha^2) = \sigma_\alpha^2,\ E(\hat{\sigma}_e^2) = \sigma_e^2. \qquad (9)$$

Eine ähnliche Beziehung für $\hat{\vartheta}$ und $\hat{\varrho}$ kann man aber nicht behaupten. Eine exakte Formel für die Varianz von $\hat{\varrho}$ ist dem Autor nicht bekannt. Der Schätzer einer Approximation von $\text{Var}(\hat{\varrho})$ für den balancierten Fall ist bei BÄTZ et al. (1972, S. 197) zu finden. In dieser Arbeit wird sowohl ein neuer Schätzer $\tilde{\varrho}$ von ϱ als auch eine Approximation von dessen Varianz vorgeschlagen. Sie beruhen auf einem besseren Schätzer $\tilde{\vartheta}$ als $\hat{\vartheta}$ von ϑ.

2. Konstruktion der Schätzer $\tilde{\vartheta}$ und $\tilde{\varrho}$

Die Unabhängigkeit der Zufallsvariablen MSE und MSA sowie die Verteilung von MSE spielen bei der Entwicklung der angekündigten Schätzer eine wesentliche Rolle. Einen Beweis dieser Unabhängigkeit sowie eine Ableitung der Verteilung

von MSE im balancierten Fall kann man in der Literatur finden, z. B. bei SCHEFFÉ (1959, S. 226). Im unbalancierten Fall wird diese Unabhängigkeit ebenso wie die Verteilung von MSE, siehe z. B. SEARLE (1971, S. 433), ohne Beweis angegeben. In den folgenden Sätzen wird dieser Fall behandelt.

Zu diesem Zweck wird das Modell (1) in Vektorform geschrieben. Die Vektoren Y und e werden, wie folgt, definiert.

$$\begin{aligned} Y &= [y_{11}, \ldots, y_{1n_1}, \ldots, y_{r1}, \ldots, y_{rn_r}]' \\ e &= [e_{11}, \ldots, e_{1n_1}, \ldots, e_{r1}, \ldots, e_{rn_r}]'. \end{aligned} \tag{10}$$

Es gilt dann:

$$Y = l\mu + Z\alpha + e, \tag{11}$$

wobei Z die Design-Matrix und

$$\alpha = [\alpha_1, \alpha_2, \ldots, \alpha_r]',$$
$$l = [1, 1, \ldots, 1]' \text{ mit } l \in R^N;$$

alle anderen Annahmen wie im Modell (1).

Wenn $A_1, \ldots, A_m$ Matrizen sind, dann bezeichnet $D(A_i)$ die Blockdiagonalmatrix

$$D(A_i) = \begin{bmatrix} A_1 & & & \\ & \ddots & & \\ & & \ddots & \\ & & & A_m \end{bmatrix} \tag{12}$$

Satz 1
Die Zufallsvariablen MSA und MSE sind stochastisch unabhängig.

Beweis
MSA und MSE lassen sich wie folgt schreiben:

$$\begin{aligned} MSA &= \frac{1}{r-1} Y' \left[D\left(n_i^{-1} l_{n_i} l'_{n_i}\right) - \frac{1}{N} ll'\right] Y \\ &= \frac{1}{r-1} Y' C_1 Y. \end{aligned} \tag{13}$$

C_1 ist die in Klammern stehende Matrix.

$$\begin{aligned} MSE &= \frac{1}{N-r} Y' \left[I_N - D\left(n_i^{-1} l_{n_i} l'_{n_i}\right)\right] Y \\ &= \frac{1}{N-r} Y' C_2 Y. \end{aligned} \tag{14}$$

C_2 ist die in Klammern stehende Matrix und

$$l_{n_i} = [1, \ldots, 1]' \text{ mit } l_{n_i} \in R^{n_i}.$$

Für die Varianz-Kovarianz-Matrix von Y gilt:

$$Var(Y) = \sigma_\alpha^2 D\left(l_{n_i} l'_{n_i}\right) + I_N \sigma_e^2 = V. \tag{15}$$

Die quadratischen Formen MSA und MSE sind stochastisch unabhängig dann und nur dann, wenn

$$C_1 V C_2 = \underline{0}. \tag{16}$$

$\underline{0}$ bezeichnet die Null-Matrix, deren Ordnung aus dem Zusammenhang zu verstehen ist.

Die Berücksichtigung der Beziehungen

$$\begin{aligned} &\left[D\left(n_i^{-1} l_{n_i} l'_{n_i}\right)\right]^2 = D\left(n_i^{-1} l_{n_i} l'_{n_i}\right) \\ &ll' D\left(n_i^{-1} l_{n_i} l'_{n_i}\right) = ll' \end{aligned} \tag{17}$$

führt leicht zu

$$\begin{aligned} C_1 V C_2 = {} & \sigma_\alpha^2 D\left(l_{n_i} l'_{n_i}\right) - \frac{\sigma_\alpha^2}{N} ll' D\left(l_{n_i} l'_{n_i}\right) \\ & + \sigma_e^2 D\left(n_i^{-1} l_{n_i} l'_{n_i}\right) - \frac{\sigma_e^2}{N} ll' \\ & - \sigma_\alpha^2 D\left(l_{n_i} l'_{n_i}\right) + \frac{\sigma_\alpha^2}{N} ll' D\left(l_{n_i} l'_{n_i}\right) \\ & - \sigma_e^2 D\left(n_i^{-1} l_{n_i} l'_{n_i}\right) + \frac{\sigma_e^2}{N} ll' \\ = {} & \underline{0}. \end{aligned} \tag{18}$$

Daraus schließt man, daß MSA und MSE stochastisch unabhängig sind.

Satz 2
Die Zufallsvariable $(N-r)MSE/\sigma_e^2$ ist χ^2-verteilt mit $(N-r)$ Freiheitsgraden.

Beweis
Y ist $N(l_\mu, V)$. Die Zufallsvariabel $(N-r)MSE/\sigma_e^2 = (Y'C_2Y)/\sigma_e^2$ ist dann und nur dann $\chi^{2\prime}\left[r(C_2), \frac{1}{2}\mu^2 l' C_2 l\right]$, wenn die Matrix $(C_2/\sigma_e^2)V$ idempotent ist (SEARLE 1971, S. 57). Es gilt:

$$(C_2V)/\sigma_e^2 = I_N - D\left(n_i^{-1} l_{n_i} l'_{n_i}\right). \tag{19}$$

Diese Matrix ist aber idempotent, wie man leicht feststellen kann. Einfach festzustellen ist auch, daß

$$C_2 l = \underline{0}. \tag{20}$$

Es gilt also:

$$(N-r)\, MSE/\sigma_e^2 \sim \chi^2 (N-r). \tag{21}$$

Ein erwartungstreuer Schätzer für ϑ ergibt sich aus $\hat{\vartheta}$, indem man einen Schätzer $\tilde{\vartheta}$ sucht, der die Form

$$\tilde{\vartheta} = c\hat{\vartheta} + d \tag{22}$$

hat und folgende Beziehung erfüllt:

$$E(\tilde{\vartheta}) = \vartheta. \tag{23}$$

Die Berücksichtigung der Sätze 1 und 2 und der Beziehung, (GRAYBILL 1976, S. 64),

$$E\left(\frac{1}{MSE\ (\nu_e/\sigma_e^2)}\right) = 1/(\nu_e - 2),\ \nu_e = N - r;\ \nu_e > 2 \tag{24}$$

führt zu den Konstanten

$$c = (\nu_e - 2)/\nu_e \text{ und } d = -2/\lambda\nu_e. \tag{25}$$

$\tilde{\vartheta}$ hat also folgende Form:

$$\tilde{\vartheta} = [(\nu_e - 2)/\nu_e](\hat{\sigma}_\alpha^2/\hat{\sigma}_e^2) - 2/\lambda\nu_e \tag{26}$$

oder

$$\tilde{\vartheta} = \frac{\nu_e - 2}{\lambda\nu_e} \cdot \frac{MSA}{MSE} - \frac{1}{\lambda}. \tag{27}$$

Der Unterschied zwischen $\tilde{\vartheta}$ und $\hat{\vartheta}$ für kleine Stichprobenumfänge ist merklich. Dieser Unterschied wird geringfügig für größere Stichprobenumfänge. Im balancierten Fall ($n_i = n$, $i = 1, \ldots, r$) hat $\tilde{\vartheta}$ die Form

$$\tilde{\vartheta}_b = \frac{r(n-1) - 2}{nr(n-1)} \cdot \frac{MSA}{MSE} - \frac{1}{n}. \tag{28}$$

Der Schätzer $\tilde{\vartheta}_b$ hat minimale Varianz, ist also der beste erwartungstreue Schätzer für ϑ, (GRAYBILL 1961, S. 378). Im allgemeinen gilt für den Schätzer $\tilde{\vartheta}$:

$$Var(\tilde{\vartheta}) < Var(\hat{\vartheta}). \tag{29}$$

Dies kann man leicht feststellen, indem man die Beziehung (26) verwendet. Es ist also klar, daß der Schätzer $\tilde{\vartheta}$ besser ist als $\hat{\vartheta}$. Die Verwendung dieses Schätzers in der Beziehung (3) führt zu dem Schätzer $\tilde{\varrho}$ von ϱ

$$\tilde{\varrho} = \tilde{\vartheta}/(1+\tilde{\vartheta}) \; . \tag{30}$$

3. Varianzen von $\tilde{\vartheta}$ und $\tilde{\varrho}$ und ihre Schätzer

Die Varianz von $\tilde{\varrho}$ läßt sich approximativ nach folgender Formel berechnen (RASCH 1976, S. 173):

$$\mathrm{Var}\left(\frac{x}{y}\right) \simeq \frac{1}{\mu_y^2}\left(\sigma_x^2 + \frac{\mu_x^2}{\mu_y^2}\sigma_y^2 - 2\frac{\mu_x}{\mu_y}\sigma_{xy}\right), \tag{31}$$

wobei $E(x) = \mu_x$, $E(y) = \mu_y$, $\mathrm{Var}(x) = \sigma_x^2$, $\mathrm{Var}(y) = \sigma_y^2$ und $\mathrm{Cov}(x, y) = \sigma_{xy}$. Die Anwendung dieser Formel für $\tilde{\varrho}$ in (30) führ zu folgendem Ergebnis:

$$\mathrm{Var}\,\tilde{\varrho} \simeq \frac{(1-\varrho)^2}{(1+\vartheta)^2}\,\mathrm{Var}\,\tilde{\vartheta} = \frac{1}{(1+\vartheta)^4}\,\mathrm{Var}\,\tilde{\vartheta}. \tag{32}$$

Für die Varianz von $\tilde{\vartheta}$ gilt:

$$\mathrm{Var}\,\tilde{\vartheta} = \left(\frac{\nu_e - 2}{\lambda\nu_e}\right)^2 \mathrm{Var}\left(\frac{\mathrm{MSA}}{\mathrm{MSE}}\right). \tag{33}$$

Aber

$$\begin{aligned}\mathrm{Var}\left(\frac{\mathrm{MSA}}{\mathrm{MSE}}\right) &= E\left(\frac{\mathrm{MSA}}{\mathrm{MSE}}\right)^2 - \left[E\left(\frac{\mathrm{MSA}}{\mathrm{MSE}}\right)\right]^2 \\ &= E\,(\mathrm{MSA})^2\,E\left(\frac{1}{\mathrm{MSE}}\right)^2 - \left[E\left(\frac{\mathrm{MSA}}{\mathrm{MSE}}\right)\right]^2 \\ &= \frac{\nu_e^2}{(\nu_e-2)\,(\nu_e-4)}\left[(\lambda^2\varkappa_3 - \varkappa_1) + \lambda^2\varkappa_4\vartheta + \lambda^2\varkappa_5\vartheta^2 + (\lambda\vartheta+1)^2\right] \\ &\quad - \left(\frac{\nu_e}{\nu_e-2}\right)^2 (\lambda\vartheta+1)^2 \; .\end{aligned} \tag{34}$$

$\varkappa_1 = 2/(N-r)$; $\varkappa_2 = -2/(N-r)\lambda$;
$\varkappa_3 = 2(N-1)/(N-r)\,(r-1)\lambda^2$;
$\varkappa_4 = 4/(r-1)\lambda$; $\varkappa_5 = 2(N^2S_2 + S_2^2 - 2NS_3)/(N^2 - S_2)^2$;
$S_2 = \sum_{i=1}^{r} n_i^2$; $S_3 = \sum_{i=1}^{r} n_i^3$.

Zu der Beziehung (34) kommt man, indem man berücksichtigt, daß

$$E\left(\frac{1}{\mathrm{MSE}}\right)^2 = \frac{\nu_e^2}{\sigma_e^4\,(\nu_e-2)\,(\nu_e-4)}\;,\; \nu_e > 4; \tag{35}$$

$$\mathrm{Var}\,(\hat{\sigma}_\alpha^2) = \varkappa_3\sigma_e^4 + \varkappa_4\sigma_e^2\sigma_\alpha^2 + \varkappa_5\sigma_\alpha^4 \quad \text{(SEARLE 1971, S. 438);} \tag{36}$$

$$\mathrm{Var}\,(\hat{\sigma}_e^2) = \varkappa_1\sigma_e^4 \quad \text{(SEARLE 1971, S. 438);} \tag{37}$$

$$\begin{aligned}E\,(\mathrm{MSA})^2 &= \mathrm{Var}(\mathrm{MSA}) + [E(\mathrm{MSA})]^2 \\ &= (\lambda^2\varkappa_3 - \varkappa_1)\,\sigma_e^4 + \lambda^2\varkappa_4\sigma_e^2\sigma_\alpha^2 + \lambda^2\varkappa_5\sigma_\alpha^4 \\ &\quad + (\lambda\sigma_\alpha^2 + \sigma_e^2)^2 \; .\end{aligned} \tag{38}$$

Die Formel für $\varkappa_3$ im Buch von SEARLE (1971, S. 438) muß korrigiert werden, indem man $(N^2 - S_2)^2$ anstelle von $(N^2 - S_2)$ schreibt.

Nach der Substitution und nach vereinfachenden Operationen erhält man für $\mathrm{Var}\,\tilde{\vartheta}$:

$$\mathrm{Var}\,\tilde{\vartheta} = b_0\vartheta^2 + b_1\vartheta + b_2, \tag{39}$$

wobei

$$b_0 = \frac{\varkappa_5(\nu_e-2)+2}{\nu_e-4}\;;\; b_1 = \frac{\lambda\varkappa_4(\nu_e-2)+4}{\lambda(\nu_e-4)}\;;$$
$$b_2 = \left(\varkappa_3 - \frac{\varkappa_1}{\lambda^2}\right)\left(\frac{\nu_e-2}{\nu_e-4}\right) + \frac{2}{(\nu_e-4)\lambda^2}\;. \tag{40}$$

Im balancierten Fall gilt:

$$\mathrm{Var}\,\tilde{\vartheta}_b = \frac{2(N-3)\,(1+n\vartheta)^2}{n^2(r-1)\,(\nu_e-4)} \tag{41}$$

Diese Varianz ist die kleinste in der Klasse der Varianzen aller unverzerrten Schätzer für ϑ.

Die approximative Varianz von $\tilde{\varrho}$ läßt sich nun nach den Beziehungen (32) und (39) wie folgt schreiben:

$$\mathrm{Var}\,\tilde{\varrho} \simeq \frac{1}{(1+\vartheta)^4}\,(b_0\vartheta^2 + b_1\vartheta + b_2). \tag{42}$$

Unter Anwendung der Beziehung

$$\mathrm{Var}\,\tilde{\vartheta} = E(\tilde{\vartheta}^2) - \vartheta^2 \tag{43}$$

in Kombination mit (39) erhält man im allgemeinen Fall einen erwartungstreuen Schätzer $\overline{\mathrm{Var}\,\tilde{\vartheta}}$ für $\mathrm{Var}\,\tilde{\vartheta}$:

$$\overline{\mathrm{Var}\,\tilde{\vartheta}} = \frac{1}{b_0+1}\,(b_0\tilde{\vartheta}^2 + b_1\tilde{\vartheta} + b_2). \tag{44}$$

Dieser Schätzer ist wiederum der beste erwartungstreue Schätzer für $\mathrm{Var}\,\tilde{\vartheta}$ im balancierten Fall (GRAYBILL 1976, S. 78).

Die Beziehungen (32) oder (42) und (44) führen zu einem Schätzer von $\mathrm{Var}\,\tilde{\varrho}$:

$$\overline{\mathrm{Var}\,\tilde{\varrho}} = \frac{1}{(1+\tilde{\vartheta})^4}\,\overline{\mathrm{Var}\,\tilde{\vartheta}}. \tag{45}$$

4. Beispiel

Daten: STAHL et al. 1969, S. 156. Die Milchfettmengenleistungen der Töchter von 10 Bullen (Tabelle 1) wurden aufgenommen. Die 10 Bullen sind eine Zufallsstichprobe aus einer bestimmten Rasse, ebenso wie die Färsen, an die sie jeweils angepaart wurden.

Tabelle 1. Milchfettmengenleistungen der Töchter von 10 Bullen

B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}
120	152	130	149	110	157	119	150	144	159
155	144	138	107	142	107	158	135	112	105
131	147	123	143	124	146	140	150	123	103
130	103	135	133	109	133	108	125	121	105
140	131	138	139	154	104	154	104	132	144
140	102	152	102	135	119	138	150	144	129
142	102	159	103	118	107	156	140	132	119
146	150	128	110	116	138	145	103	129	100
130	159	137	103	150	147	150	132	103	115
152	132	144	138	148	152	124	128	140	146
115	102	154	–	138	124	100	122	106	108
146	160	–	–	115	142	–	154	152	119
12	12	11	10	12	12	11	12	12	12

Aus den Daten der Tabelle 1 wird folgende einfache Varianzanalyse aufgestellt:

Tabelle 2. Einfache Varianzanalyse

Varianzursache	SS (Quadratsumme)	df (Freiheitsgr.)	MS (Mittelquadrats.)
Zwischen den Bullen	SSA = 3609,15	9	MSA = 401,02
Innerhalb der Bullen	SSE = 33426,05	106	MSE = 315,34
Gesamt	SST = 37035,20	115	–

Nach den Formeln (5) und (6) ergibt sich:

$\lambda = 11{,}596$, $\hat{\sigma}_e^2 = 315{,}34$, $\hat{\sigma}_\alpha^2 = 7{,}389$.

Für den Schätzer $\tilde{\vartheta}$ ergibt sich nach der Formel (27)

$\tilde{\vartheta} = 0{,}021$.

Die Koeffizienten $\varkappa_1, \ldots, \varkappa_5$, die unmittelbar der Beziehung (34) folgen, sind:

$\varkappa_1 = 0{,}019$; $\varkappa_2 = -0{,}002$; $\varkappa_3 = 0{,}002$; $\varkappa_4 = 0{,}038$;
$\varkappa_5 = 0{,}223$.

Mit Hilfe dieser Koeffizienten lassen sich die Koeffizienten b_0, b_1 und b_2 in (40) berechnen.

$b_0 = 0{,}247$; $b_1 = 0{,}042$; $b_2 = 0{,}002$

Die Schätzwerte für Var $\tilde{\vartheta}$ und Var $\tilde{\varrho}$ lassen sich aus den Beziehungen (44) und (45) errechnen.

$\overline{\text{Var } \tilde{\vartheta}} = 0{,}002$; $\overline{\text{Var } \tilde{\varrho}} = 0{,}002$.

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Anschrift des Verfassers: Dipl.-Math. Dr. E. Stavrakakis, Central Health Council, Aristotelous 19, 10187 Athens, Greece

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How to differentiate between impact and effect using BOX and TIAO intervention functions: some zero and first order cases

M. G. Schimek

Summary

Single-case quasi-experimental designs are generally accepted in evaluation research (e.g. COOK and CAMPBELL, 1979). For time dependent data of at least interval-scale level, two statistical techniques for the assessment of potential impacts are known but not widely adopted. In economics and technology the approach of BOX and TIAO (1975) dominates. In the social sciences, especially in education and psychology, the method of GLASS, WILLSON and GOTTMAN (1975) is prefered. For historical reasons both techniques have developed quite independently. In medicine and biology they are almost unknown in spite of their potential in evaluating change in the single-case context.

In this article we briefly describe and compare both approaches, pointing out that they are conditionally equivalent. We define demands for statistical techniques to cope well with the need for impact assessment in psychology, medicine and biology. It is shown that the BOX and TIAO intervention model can be applied in a non-standard way to meet the demands specified. On the input side of the intervention (transfer) function we distinguish event and process impact variables. This allows the analyst to see how intervention functions interact with the impact quality and duration and to study characteristic outputs in terms of intervention effects. As a result we are in the situation to differentiate between impact and effect of an intervention in an univariate (single-case) problem. Some zero and first order intervention functions are discussed and their behaviour is studied.

Zusammenfassung

Einzelfallbezogene quasiexperimentelle Designs sind in der Evaluationsforschung allgemein anerkannt (e.g. COOK and CAMPBELL, 1979). Für zeitabhängige Daten von zumindest Intervallskalenniveau sind zwei statistische Techniken für die Abschätzung von potentiellen Einflüssen bekannt, werden aber nicht häufig angewendet. In der Ökonomie und der Technik dominiert der Ansatz von BOX and TIAO (1975). In den Sozialwissenschaften, insbesondere in der Pädagogik und der Psychologie, wird die Methode von GLASS, WILLSON and GOTTMAN (1975) bevorzugt. Aus historischen Gründen haben sich beide Techniken recht unabhängig entwickelt. In der Medizin und der Biologie sind sie, im Gegensatz zu ihrem Potential, Änderungen im Einzelfallkontext zu evaluieren, fast unbekannt.

In diesem Artikel beschreiben und vergleichen wir kurz beide Ansätze, wobei wir darauf hinweisen, daß sie bedingt äquivalent sind. Wir definieren Anforderungen an statistische Techniken, um dem Bedarf nach Einflußabschätzung in der Psychologie, Medizin und Biologie genügend nachzukommen. Es wird gezeigt, daß durch eine nicht-standardmäßige Anwendung des BOX and TIAO Interventionsmodells die spezifizierten Anforderungen erfüllt werden können. Bei der Inputseite der Interventions-(Transfer-)funktion unterscheiden wir zwischen Ereignis- und Prozeß-Einflußvariablen. Dies erlaubt dem Untersucher zu erkennen, wie Interventionsfunktionen mit der Einflußqualität und -dauer interagieren und charakteristische Outputs in Form von Interventionseffekten zu studieren. Als Ergebnis sind wir in der Lage, bei einem univariaten (Einzelfall-)Problem zwischen Einfluß und Wirkung einer Intervention zu unterscheiden. Einige Interventionsfunktionen nullter und erster Ordnung werden diskutiert und ihr Verhalten studiert.

1. The GLASS, WILLSON and GOTTMAN approach

GLASS, WILLSON and GOTTMAN's approach is an extension of the generalized least square technique introduced by AITKEN (1935).

We have a regression problem

$$\underline{y} = \underline{X}\,\underline{\beta} + \underline{\varepsilon} \qquad (1)$$

where $\underline{y}$ is a Tx1 vector of observations on the dependent variable, $\underline{\beta}$ is a Kx1 vector of unknown coefficients, $\underline{X}$ is a TxK ($T \geq K$) nonstochastic matrix of rank K of observations on the explanatory variables (design matrix) and $\underline{\varepsilon}$ is a Tx1 vector of random errors with $E(\underline{\varepsilon}) = \underline{0}$ and $E(\underline{\varepsilon}\,\underline{\varepsilon}^T) = \sigma^2\,\underline{\Omega}$, $\underline{\Omega}$ being a known covariance matrix (symmetric, positive definite). Moreover, as the sample size T becomes infinitely large it is assumed that

$$\lim_{T\to\infty} (\underline{X}^T\,\underline{\Omega}^{-1}\underline{X}/T) = \underline{Q}_\Omega$$

where $\underline{Q}_\Omega$ is a finite and nonsingular matrix (SEBER, 1977, 60 pp.). The generalized least square model differs from the

ordinary least square model as in the latter the covariance matrix is the identity matrix $\underline{I}$. In ordinary least squares the errors are assumed to be independent random variables. In practice the covariance matrix is not known when the errors are dependent. It can only be estimated for some simplified structures. GASS, WILLSON and GOTTMAN (1975) have proposed some design matrices for specific error processes in a time series context to make a generalized least square estimation feasible.

Let us assume an ARIMA (p, d, q) noise (error) model. For the general nonstationary time series case we define the backshift operator B such that $Bn_t = n_{t-1}$, where n_t are equally spaced observations representing the noise in the time domain. Further we suppose a random variable a_t of independent and identically distributed random shocks. Now an ARIMA model of order (p, d, q) can be expressed as (»general form« in the notation of BOX and JENKINS, 1976, 91 pp.)

$$n_t = \frac{\Theta_q(B)}{(1-B)^d\,\Phi_p(B)}\,a_t + \frac{\theta_o}{\Phi_p(B)\,(1-B)^d} \qquad (2)$$

with the autoregressive operator of order p

$$\Phi_p(B) = (1 - \varphi_1 B - \varphi_2 B^2 - \ldots - \varphi_p B^p),$$

the moving average operator of order q

$$\Theta_q(B) = (1 - \theta_1 B - \theta_2 B^2 - \ldots - \theta_q B^q)$$

and θ_o an unknown constant (often set to zero). It is assumed that the roots of $\Phi_p(B) = 0$ lie outside the unit circle (stationary autoregressive operator). GLASS, WILLSON and GOTTMAN (1975) introduce a parameter

$$L = \frac{\theta_o}{\Phi_p(B)\,(1-B)^d}\,.$$

Thus we can write (2) as

$$n_t - L = \frac{\theta_q(B)}{\Phi_p(B)\,(1-B)^d}\,a_t \qquad (3)$$

and the deviation $(n_t - L)$ can be understood as an infinite moving average process for $d > 0$ and/or $p > 0$. According to BOX and JENKINS (1976, p. 9) we define the linear operator

$$\Psi(B) = (1 + \psi_1 B + \psi_2 B^2 + \ldots)$$

which is called the transfer function with weights ψ_i of the linear filter transforming white noise a_t to the noise process n_t. Now (3) can be written as

$$n_t - L = \frac{\Theta_q(B)}{\Phi_p(B)\,(1-B)^d}\,a_t = \Psi(B)\,a_t \qquad (4)$$

and we finally have

$$n_t = L + \sum_{j=0}^{\infty} \psi_j\, a_{t-j}.$$

This is what BOX and JENKINS (1976, p. 95) call the »random shock form« of the stochastic model.

After some algebra equation (4) takes the form

$$\Theta_q(B)a_t = \Phi_p(B)\,(1-B)^d\,\Psi(B) = \varphi(B)\,\Psi(B)a_t$$

where $\varphi(B) = \Phi(B)\,(1-B)^d$ is the generalized autoregressive operator, in which one or more of the roots of $\varphi(B) = 0$ lie on the unit circle (BOX and JENKINS, 1976, p. 11). The operator equation

$$\Theta_q(B) = \varphi(B)\,\Psi(B)a_t$$

allows to evaluate the unknown weights ψ_i by equating the coefficients of powers of B (BOX and JENKINS, 1976, 95 p.).

GLASS, WILLSON and GOTTMAN (1975) consider in their approach a time-dependent linear regression model (extension of (1) under the same assumptions)

$$\underline{y} = \underline{X}\,\underline{\beta} + \underline{\Psi}\,\underline{a} \qquad (5)$$

where $\underline{X}$ is a design matrix which models the intervention effects. Moreover $\underline{\varepsilon} = \underline{\Psi}\;\underline{a} = \Psi(B)\;\underline{a}$ and $\underline{\Psi}$ is an operator matrix of the linear operator B. Because the errors ε_t are not independent any more, we have

$$E\,(\underline{\varepsilon}\;\underline{\varepsilon}^T) \neq \sigma_\varepsilon^2\,\underline{I}.$$

Due to the specific choice of error process, the dispersion of the correlated errors ε_t is known and given by

$$E\,(\underline{\varepsilon}\;\underline{\varepsilon}^T) = \sigma_a^2\,\underline{\Omega} = \sigma_a^2 \cdot$$

	1	2	3		1		∞
1	ψ_o^2	$\psi_o\psi_1$	$\psi_o\psi_2$	⋯	$\psi_o\psi_{l-1}$	⋯	$\psi_o\eta$
2	$\psi_o\psi_1$	$\psi_o^2 + \psi_1^2$	$\sum_{i=1}^{2} \psi_{2-i}\psi_{3-i}$	⋯	$\sum_{i=1}^{2} \psi_{2-i}\psi_{l-i}$	⋯	$\eta \sum_{i=1}^{2} \psi_{2-i}$
3	$\psi_o\psi_2$	$\sum_{i=1}^{2} \psi_{2-i}\psi_{3-i}$	$\sum_{i=1}^{3} \psi_{i-1}^2$	⋯	$\sum_{i=1}^{3} \psi_{3-1}\psi_{l-i}$	⋯	$\eta \sum_{i=1}^{3} \psi_{3-i}$
4	$\psi_o\psi_3$	$\sum_{i=1}^{2} \psi_{2-i}\psi_{4-i}$	$\sum_{i=1}^{3} \psi_{3-i}\psi_{4-i}$	⋯	$\sum_{i=1}^{4} \psi_{4-i}\psi_{l-i}$	⋯	$\eta \sum_{i=1}^{4} \psi_{4-i}$
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
k	$\psi_o\psi_{k-1}$	$\sum_{i=1}^{2} \psi_{2-i}\psi_{k-i}$	$\sum_{i=1}^{3} \psi_{3-i}\psi_{k-i}$	⋯	$\sum_{i=1}^{\min\{k,l\}} \psi_{k-i}\psi_{l-i}$	⋯	$\eta \sum_{i=1}^{k} \psi_{k-i}$
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
∞	$\psi_o\eta$	$\eta \sum_{i=1}^{2} \psi_{2-i}$	$\eta \sum_{i=1}^{3} \psi_{3-i}$	⋯	$\eta \sum_{i=1}^{l} \psi_{l-i}$	⋯	$\sum_{i=1}^{\infty} \psi_{i-1}^2$

where $\eta = \lim_{j\to\infty} \psi_j$ and the weights ψ_j are computable (GLASS, WILLSON and GOTTMAN, 1975, 153 p.). MÖBUS, GÖRICKE and KRÖH (1983, 107 p.) provide for a straight forward derivation of these weights.

The operator matrix $\underline{\Psi}$ is (TxT) and for the triangular form

$$\underline{\Psi} = \begin{bmatrix} 1 & & & & \\ \psi_1 & 1 & & & \\ \psi_2 & \psi_1 & 1 & & 0 \\ \vdots & \ddots & \ddots & \ddots & \\ \psi_{T-1} & \cdots & \psi_2 & \psi_1 & 1 \end{bmatrix}$$

Thus $\underline{\Psi}^{-1} = \sum_{i=0}^{u} (\underline{I} - \underline{\Psi})^i$

for $u \ll \infty$ and we can write (5) as

$$\underline{\Psi}^{-1}\,\underline{Y} = \underline{\Psi}^{-1}\underline{X}\,\underline{\beta} + \underline{a} \text{ and}$$
$$\underline{Y}^* = \underline{X}^*\,\underline{\beta} + \underline{a}\,.$$

Finally the time-dependent regression model with correlated errors can be converted into one with uncorrelated errors by applying the recursive relationships

$$y_t^* = y_t - \sum_{i=1}^{t-1} \psi_i\, y_{t-i}^*\,,$$
$$x_{tk}^* = x_{tk} - \sum_{i=1}^{t-1} \psi_i\, x_{t-i,k}^* \text{ and}$$
$$a_t = \varepsilon_t - \sum_{i=1}^{t-1} \psi_i\, \alpha_{t-i}\,.$$

Now an ordinary least square estimation applies. For the proof of the recursion and for the estimation procedure we refer to GLASS, WILLSON and GOTTMAN (1975) and GOTTMAN (1981).

2. The BOX and TIAO approach

The approach of BOX and TIAO (1975) is not an extension of the generalized least square technique. It is based on the linear transfer function model by BOX and JENKINS (1976, 345 pp.).

Again we suppose equally spaced time dependent observations, but now in pairs (X_t, Y_t), X_t being the input and Y_t being the output of a linear dynamic system. The general form of a transfer function model of order (r, s) is given by

$$\delta_r(B)\, Y_t = \omega_s(B)\, X_{t-b}$$

with two polynomials in B

$$\delta_r(B) = (1 - \delta_1 B - \delta_2 B^2 - \ldots - \delta_r B^r)$$

and

$$\omega_s(B) = (\omega_o - \omega_1 B - \omega_2 B^2 - \ldots - \omega_s B^s)$$

and a parameter b indicating the discrete system lag.

The stability of the linear dynamic system is guaranteed when the roots of $\delta_r(B) = 0$ lie outside the unit circle (compare with the stationarity condition of the ARIMA (p, d, q) model). The transfer function operator is defined by

$$v(B) = (v_o + v_1 B + v_2 B^2 + \ldots) = \frac{\omega_s(B)B^b}{\delta_r(B)} = \frac{\Omega(B)}{\delta(B)}$$

where the sequence of weights $v_o, v_1, v_2, \ldots$ is called the impulse response function. The transfer function is the ratio of the polynomial $\Omega(B)$ over the polynomial $\delta(B)$.

In the BOX and TIAO (1975) approach we have an intervention (transfer function) model with a noise process as specified in (4)

$$Y_t = \frac{\Omega(B)}{\delta(B)}\, I_t + L + \psi(B)\, a_t$$

with a special (indicator) variable I_t instead of the general input variable X_t. The intervention model, as being linear in its components, can be decomposed to

$$Y_t - L = S_t + N_t \qquad (6)$$

where S_t is the systematic (deterministic) intervention component and N_t the noise (stochastic) component.

BOX and TIAO (1975, p. 71) introduce an indicator variable to model potential intervention effects. They differentiate two types of indicator variables, the step variable

$$I_t^{(s)} = \begin{cases} 0 \text{ for } t < T^{(I)} \\ 1 \text{ for } t \geq T^{(I)} \end{cases}$$

and the pulse variable

$$I_t^{(p)} = \begin{cases} 0 \text{ for } t \neq T^{(I)} \\ 1 \text{ for } t = T^{(I)} \end{cases}$$

where $T^{(I)}$ is the first observation point not belonging to the preintervention series (belongs to the so called postintervention series which is a missleading term and should not be used). By differencing the step variable the pulse variable can be obtained: $I_t^{(p)} = (1 - B)\, I^{(s)}{}_t$.

The choice of the intervention function which we define as

$$f(I_t) = \frac{\omega_s(B)B^b}{\delta_r(B)} = \frac{\Omega(B)}{\delta(B)}$$

is unrestricted. Although, BOX and TIAO (1975, 71 p.) suggest applying zero order functions (order of $\delta(B)$ is zero) like

$$f(I_t) = \omega_o\, B^b\, I_t$$

or first order functions (order of $\delta(B)$ is one) like

$$f(I_t) = \frac{\omega_o\, B^b}{1 - \delta_1 B}\, I_t\,.$$

In the latter the parameter δ_1, which can be interpreted as rate parameter, has to be less than one for stability reasons.

The intervention model is a special case of the transfer function model and can be calculated exactly in the same way. For the details of the nonlinear least square estimation we refer to BOX and JENKINS (1976, 390 p.) and BOX and TIAO (1975, 72 p.).

3. Comparison in the light of conditional equivalence

For the comparison of the two discussed approaches for intervention analysis it is valuable to know that the GLASS, WILLSON and GOTTMAN (1975) model is conditionally equivalent to that of BOX and TIAO (1975), as MÖBUS, GÖRICKE and KRÖH (1983) have shown.

Again we consider equation (5), writing

$$y_t = f_t(L, \beta_1, \beta_2, \ldots, \beta_{s+1}) + \psi(B)\, a_t,$$

where f_t is a function of the intervention parameters and

$$y_t = \frac{\Omega(B)}{\delta(B)}\, I_t + L + \psi(B)\, a_t$$

is the single observation equation of the GLASS, WILLSON and GOTTMAN and the BOX and TIAO approach, respectively (L under the theoretical assumption of a nontruncated white noise process). Ignoring $\psi(B)a_t$, one has to show that for fixed parameters δ_i $(i = 1, 2, \ldots, r)$ of $\delta(B)$ and $s + 1$ intervention parameters β_j both sides of the equation

$$S_t + L = f_t\,(L, \beta_1, \beta_2, \ldots, \beta_{s+1})$$

are equivalent. MÖBUS, GÖRICKE and KRÖH (1983, 105 p.) show that S_t can always be expressed as

$$S_t = [g_{t,1} \quad g_{t,2} \quad \cdots \quad g_{t,s+1}] \begin{bmatrix} \omega_o \\ -\omega_1 \\ \vdots \\ -\omega_s \end{bmatrix} \qquad \forall\ t > T + b,$$

where

$$g_{t,k} = I_{t-b-k+1} + \sum_{i=1}^{r} \delta_i\, g_{t-i,k}$$

and $g_{t,k} = 0$ for $t \leq T + b + k - 1$. Because of the a priori known δ_i (assumption) the elements $g_{t,k}$ are fixed and provide all the information needed to model the intervention effects (in the design matrix $\underline{X}$). As a result of this, the equivalence holds. Moreover both models can be interpreted as extensions of the generalized least squares model.

4. Demands for impact assessment techniques and how they are met

We refine ourselves to single-case quasi-experimental designs in the context of time series analysis. This research strategy is discussed extensively in COOK and CAMPBELL (1979), in KRATOCHWILL (1978) and in GOTTMAN and GLASS (1978). In general our evaluation problem can be described as follows: Let us have a time series $y_1, y_2, \ldots, y_{T-1}^{(I)}, y_T^{(I)}, y_{T+1}^{(I)}, \ldots, y_{T-1}, y_T$, where the y_t are equally spaced observations of at least interval-scale level made on the behaviour of some subject (single-case). This series is a time sample of length T representing an underlying population process (in the time domain). Further it is understood that a specific impact – technically speaking an intervention – operates on the process. It is this intervention we want to assess by the means of impact assessment techniques. Generally we are assuming that at least the onset of the impact is known. In the quasi-experimental design we call the starting point of the intervention $T^{(I)}$. Although it is desirable to have further prior information on the intervention as duration and relative intensity, when the impact is not a single event.

Based on these assumptions we formulate a list of demands which should be met by an adequate intervention assessment technique. It should allow

(1) to differentiate between the intervention impact as represented in the exogenous intervention variable and the intervention effect being observed in the time series;
(2) for a great variety of both event and process type intervention inputs (exogenous variables) to provide for the possibility to model different impact structures;
(3) for some well-defined class of operations which transform the intervention impact (input) in an intervention effect (output);
(4) for a straight forward statistical evaluation based on an estimation procedure already applied in time series analysis;
(5) to make use of all prior information available on the exogenous variables in a quasi-experimental design context;
(6) to evaluate interventions even when the preintervention (baseline) series have few observations as long as there is sufficient prior information on the baseline process involved;
(7) to test for the existence, the effect structure (shape) and the time structure (behaviour) of interventions and
(8) to analyse overlapping effects of combined intervention impacts (more than one intervention variable).

As can easily be seen from the outline of the approaches of GLASS, WILLSON and GOTTMAN and BOX and TIAO, non of them meets the basic demand to differentiate between intervention impact and intervention effect but it will be shown that the latter can be adapted appropriately.

It is worthwhile to point out that the technique of GLASS, WILLSON and GOTTMAN suffers from a fundamental problem. That is, you have to model the intervention effect through the design matrix. This does not only mean an extensive need for prior information on the effects but also that you are strictly speaking unable to test any intervention hypothesis. The procedure allows only to simulate effects for a restricted class of presumed effect structures (design matrices) under a least squares criterion. It does not permit the estimation of rate parameters (see conditional equivalence). Although, rate effects can be modelled in the design matrix (due to GLASS, WILLSON and GOTTMAN the design matrix is not restricted to elements 0 and 1). Obviously this does not overcome its basic shortcomings and inflexibility nor the fact that the estimation procedure is a standard one. Which demands are met by the approach of GLASS, WILLSON and GOTTMAN (abbreviated GWG) can be seen from Table 1.

Table 1. Demands for impact assessment techniques and how they are met by GLASS, WILLSON and GOTTMAN (1975; GWG), BOX and TIAO (1975; BT) and modified BOX and TIAO (MBT)

Demand	Approach		
	GWG	BT	MBT
(1) Differentiation between impact and effect	no	no	yes
(2) Event and process input	yes	no	yes
(3) Class of transformation operations	no	yes	yes
(4) Time series estimation procedure	no	yes	yes
(5) Prior information in quasi-experimental design	yes	no	yes
(6) Preintervention series dispensable	no	no	yes
(7) Test of existence, effect and time structure	no	yes	yes
(8) Analysis of overlapping effects	no	yes	yes

The approach of BOX and TIAO can be remedied for not meeting the first demand and as a result of this also the second. As proposed by its authors it makes use of the well-defined class of transfer functions. This also means straight forward estimation procedures used in time series analysis. The technique is already outlined in a way to account for different degrees of prior information and allows for quasi-experimental design methodology. It should also be stressed that it allows to test the existence, the effect structure and the time structure to a great extend. Furthermore it is designed to cope with more than one intervention variable as being an extension of the BOX and JENKINS (1976) transfer function models (multivariate). The demands satisfied by the BOX and TIAO approach (abbreviated BT) are shown in Table 1.

5. How to differentiate between intervention impact and intervention effect in the Box and Tiao approach

In evaluation research it is very much desirable, firstly, to make use of the full prior information available on the exogenous intervention variable or variables, secondly, to obtain a stochastic answer about tentative models which relate impact

data to potential effects in the observed data (time series), and thirdly, to do inference on hypotheses concerning existence, shape and behaviour of intervention effects. This means that it is essential to differentiate between intervention impacts on the input and intervention effects on the output side. Fortunately there is a straight forward way to answer this demand. The basic idea is to classify the impact data and to map them onto certain intervention variables. This drastically reduces the number of potential intervention functions for a given class of effects in the observed series. By estimating and testing relevant intervention functions in a sequence we can find an appropriate impact assessment model under minimum residual sum of squares and parsimony considerations.

In addition to the assumptions made in chapter 4, we assume that the features of the noise process remain unchanged for the period of analysis, the intervention model is linear in its components, the deterministic component dominates at least at one time point the noise component and that there is no shift in the (constant) variance of the time series.

Let us again consider the intervention model (6)

$$Y_t - L = S_t + N_t$$

with $S_t = f(I_t)$, the systematic component being a function f of a variable I_t which we call intervention variable (i.e. an intervention function). BOX and TIAO (1975) reduce themselves to indicator variables $I_t \in \{0,1\}$ to model intervention effects directly. We also make use of such discrete event variables – event happens or not – but to represent the intervention impacts. Moreover we propose continuous intervention variables of the type $I_t \in [0,1] \cap Q$ (Q the rational numbers), which we call process variables – a process of changing intensity realizes. The latter represent a continuous process as a sequence of events in a discretized way.

Further we do not only classify the intervention impact according to its quality – event or process – but also according to its duration. We differentiate between an instantaneous, temporary and permanent occurrence of an impact. For practical reasons we consider only finite intervention impacts and effects. This is guaranteed by the condition

$$\sum_{t=1}^{\infty} | I_t | < C,$$

where C is a finite constant.

Under these assumptions we can define five different types of intervention variables.

Table 2 shows that for a given duration these intervention variables are related to each other. In the instantaneous case one cannot define a process type variable but in all other instances the event type variable is always a special case of the process type variable as 1 is element of the interval $(0,1] \cap Q$. Thus the intervention variables $I_t^{(2)}$ and $I_t^{(4)}$, $I_t^{(3)}$ and $I_t^{(5)}$ are related, respectively. The above classification enables us to account for all feasible types of impact which can be studied in a single-case time domain context.

Let us now assume that an intervention variable is given, either observed or fixed for a defined quasi-experimental design. Then we are in the position to systematically describe the behaviour of certain classes of intervention functions in terms of effects. As we want to apply the BOX and TIAO approach, we restrict ourselves to their intervention (transfer) functions. For simplicity we shall be confined to zero and first order functions with level parameters only. From a practical point of view they are also discussed by MCCLEARY and HAY (1980, 141 pp.), although they do not propose a method to differentiate between impact and effect. Our intervention model (6) is linear in its components and we can subtract both the constant L and the noise N_t without any loss of generality. This results in

$$Y_t^* = S_t = f(I_t) \qquad (7)$$

which is more convenient for further investigation. This equation allows us to evaluate the behaviour of the intervention function f in dependence of any event or process type intervention variable analytically.

In engineering equation (7) is known as a linear system in the time domain and written $y_t = \sum_{k=-\infty}^{+\infty} h_k x_{t-k}$ where $\{h_k\}$ is the impulse response function with $h_k = 0$ for $k < 0$ (causal). The system is linear if, and only if, a linear combination of inputs $\lambda_1 x_1(t) + \lambda_2 x_2(t)$ (λ_1, λ_2 constants) produces the same linear combination of outputs, which is $\lambda_1 y_1(t) + \lambda_2 y_2(t)$. Moreover time-invariance is assumed, which means that a delay of time τ in the input brings about the same delay in the output (CHATFIELD, 1984, 186 p.).

For event type intervention variables we trivially have a discrete system. In the process type case we study a continuous phenomenon in a descretized way and again end up with a discrete system.

6. The zero-order intervention function in one level parameter and its behaviour

The zero-order (highest power of B is zero) intervention function is defined as

$$f(I_t) = \omega_0 I_t \qquad (8)$$

Table 2. Classification of intervention variables according to the quality and duration of impact

		Quality: event	Quality: process
Duration	instantaneous	$I_t^{(1)} = \begin{cases} 0 \text{ for } t < T^{(I)1)} \\ 1 \text{ for } t = T^{(I)} \\ 0 \text{ for } t > T^{(I)} \end{cases}$	undefined
	temporary	$I_t^{(2)} = \begin{cases} 0 \text{ for } t < T^{(I)} \\ 1 \text{ for } T^{(I)} \le t < T^{(I)} + d^{2)} \\ 0 \text{ for } t \ge T^{(I)} + d \end{cases}$	$I_t^{(4)} = \begin{cases} 0 & \text{for } t < T^{(I)} \\ p_t^{3)} & \text{for } T^{(I)} \le t < T^{(I)} + d \\ 0 & \text{for } t \ge T^{(I)} + d \end{cases}$
	permanent	$I_t^{(3)} = \begin{cases} 0 \text{ for } t < T^{(I)} \\ 1 \text{ for } t \ge T^{(I)} \end{cases}$	$I_t^{(5)} = \begin{cases} 0 & \text{for } t < T^{(I)} \\ p_t & \text{for } t \ge T^{(I)} \end{cases}$

1) $T^{(I)}$ denotes the onset of the impact.
2) d denotes the impact duration counted in discrete points of time.
3) p_t denotes the intensity of an intervention process and takes the values $p_t \in (0,1] \cap Q$

where ω_o is an unrestricted level parameter depending on the scale of the observed endogenous (time series) variable. The parameter allows for different effect shapes.

Given an instantaneous event type intervention variable $I_t^{(1)}$, equation (7) for a zero-order intervention function (8) becomes

$$Y_t^* = \omega_o I_t^{(1)}.$$

For $t < T^{(I)}$ prior to the event we have

$$I_i = 0 \text{ and } Y_i^* = \omega_o 0 = 0,$$

for $t = T^{(I)}$ at the event (let $i = T^{(I)} + 1$)

$$I_{i+1} = 1 \text{ and } Y_{i+1}^* = \omega_1 1 = \omega_o$$

and then for $t > T^{(I)}$ we obtain (let $i + n = T$)

$$\begin{aligned} I_{i+2} &= 0 \text{ and } Y_{i+2}^* = \omega_o 0 = 0 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= 0 \qquad Y_{i+n}^* = \omega_o 0 = 0. \end{aligned}$$

The given sequence of inputs $I_t^{(1)}$ in combination with the function (8) can only produce a single pulse effect ω_o at $T^{(I)}$.

Let us now consider a temporary event type intervention variable $I_t^{(2)}$ together with equation (7) and function (8). That is

$$Y_t^* = \omega_o I_t^{(2)}.$$

For $t < T^{(I)}$ before the onset of the event

$$I_i = 0 \text{ and } Y_i^* = \omega_o 0 = 0.$$

For $T^{(I)} \leq t < T^{(I)} + d$ during the event we have (let $i = T^{(I)} + 1$)

$$\begin{aligned} I_{i+1} &= 1 \text{ and } Y_{i+1}^* = \omega_o 1 = \omega_o \\ &\vdots \qquad\qquad \vdots \\ I_{i+m} &= 1 \qquad Y_{i+m}^* = \omega_o 1 = \omega_o \end{aligned}$$

and afterwards for $t \geq T^{(I)} + d$ (let $i + n = T$)

$$\begin{aligned} I_{i+m+1} &= 0 \text{ and } Y_{i+m+1}^* = \omega_o 0 = 0 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= 0 \text{ and } Y_{i+n}^* = \omega_o 0 = 0. \end{aligned}$$

The sequence of inputs $I_t^{(2)}$ together with the function (8) yields a temporary constant step effect starting at $T^{(I)}$.

Having a permanent event type intervention variable $I_t^{(3)}$ in combination with a zero-order intervention function (8), equation (7) is

$$Y_t = \omega_o I_t^{(3)}.$$

For $t < T^{(I)}$ before the onset of the event

$$I_i = 0 \text{ and } Y_i^* = \omega_o 0 = 0.$$

From the occurence of the event onwards we obtain (let $i + 1 = T^{(I)}$ and $i + n = T$)

$$\begin{aligned} I_{i+1} &= 1 \text{ and } Y_{i+1}^* = \omega_o 1 = \omega_o \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= 1 \qquad Y_{i+n}^* = \omega_o 1 = \omega_o. \end{aligned}$$

In this instance we have a result similar to the last one but of permanent duration.

The cases considered yet allow for primitive intervention effects only. Primitive means that only simple shapes which do not depend on previous values of the intervention variable, once the event has occured, can be modelled. Although these cases can be of practical value, especially if somebody wants to test the mere existence of an intervention effect. The input assumed till now is that of a minimal information to carry out any evaluation research. Especially in the biosciences intervention impacts usually cannot be expected to be representable by indicator variables. That is why we propose process variables to represent impacts of changing intensity. To assume event instead of process type variables in biosystems always means a critical simplification. For the purpose of better evaluation research we should apply process variables as long as appropriate prior information is available.

Given a temporary process type intervention variable $I_t^{(4)}$, equation (7) for a zero-order intervention function (8) takes the form

$$Y_t^* = \omega_o I_t^{(4)}.$$

For $t < T^{(I)}$ prior to the impact process it is

$$I_i = 0 \text{ and } Y_i^* = \omega_o 0 = 0$$

and then for $T^{(I)} \leq t < T^{(I)} + d$ during it (let $i + 1 = T^{(I)}$)

$$\begin{aligned} I_{i+1} &= p_1 \text{ and } Y_{i+1}^* = \omega_o p_1 \\ I_{i+2} &= p_2 \qquad Y_{i+2}^* = \omega_o p_2 \\ &\vdots \qquad\qquad \vdots \\ I_{i+m} &= p_m \qquad Y_{i+m}^* = \omega_o p_m. \end{aligned}$$

For $t \geq T^{(I)} + d$ ($d = m + 1$) when the impact process has died out we have (let $i + n = T$)

$$\begin{aligned} I_{i+m+1} &= 0 \text{ and } Y_{i+m+1}^* = \omega_o 0 = 0 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= 0 \qquad Y_{i+n}^* = \omega_o 0 = 0. \end{aligned}$$

As can easily be seen, this combination of a sequence of inputs $I_t^{(4)}$ and the function (8) allows for a wide variety of effects of changing intensity (shape) in dependence of the given values p_t which are positive and less equal one. Thus the maximal effect occurs for $p_t = 1$ and is equal to the value of the level parameter ω_o (positive or negative). The effect only lasts for d time units.

Finally we assume a permanent process type intervention variable I_t together with a zero-order intervention function (8). Equation (7) is given by

$$Y_t^* = \omega_o I_t^{(5)}.$$

For $t < T^{(I)}$ before the impact process occures we have

$$I_i = 0 \text{ and } Y_i^* = \omega_o 0 = 0.$$

From the onset of the impact process onwards, this is for $t \geq T^{(I)}$, we have the following results (let $i + 1 = T^{(I)}$)

$$\begin{aligned} I_{i+1} &= p_1 \text{ and } Y_{i+1}^* = \omega_o p_1 \\ I_{i+2} &= p_2 \qquad Y_{i+2}^* = \omega_o p_2 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= p_n \qquad Y_{i+n}^* = \omega_o p_n. \end{aligned}$$

This case differs from the previous one in that it allows to model effects which at least go on for the period under investigation. All other considerations are exactly the same as carried out above.

For the purpose of illustration Figure 1 displays an example for each case discussed above. Moreover Figure 1 helps to classify empirial intervention effects in terms of specific inputs together with certain functions.

The potential of analysing intervention effects can be extended to a great deal by considering first-order intervention functions which take the current and the previous impact into account.

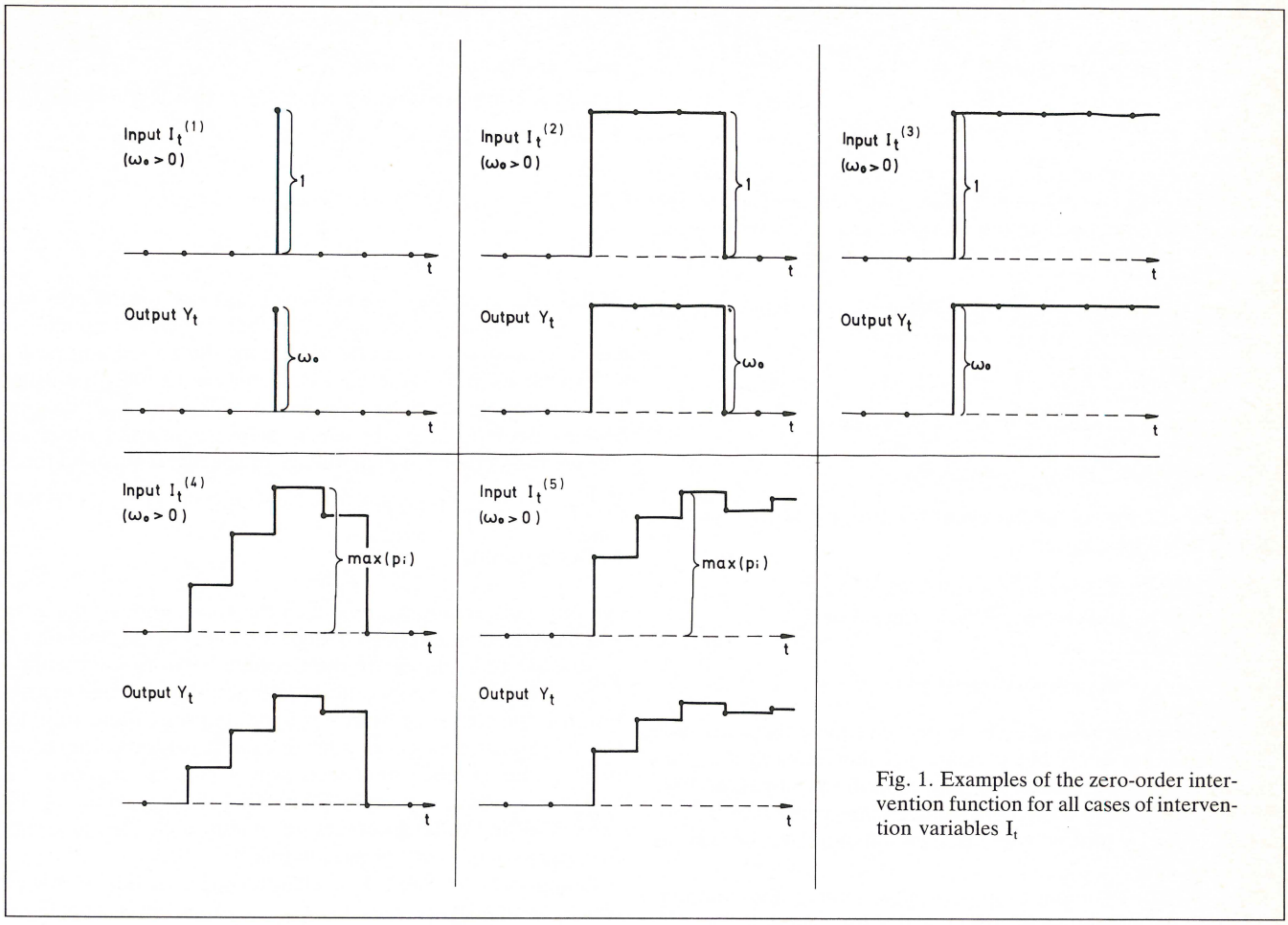

Fig. 1. Examples of the zero-order intervention function for all cases of intervention variables I_t

7. The first-order intervention function in two level parameters and its behaviour

The simplest first-order intervention function is that in two level parameters. It is given by

$$f(I_t) = (\omega_o - \omega_1 B)\, I_t. \qquad (9)$$

It is of first order because the highest power of B is one. B operates on the parameter ω_1. Thus ω_1 is a level parameter which weights the previous intervention impact (lag one) and is unrestricted. The parameter ω_o gives weight to the current intervention impact (unlaged) and is unrestricted too. Both level parameters depend on the scale of the observed endogenous (time series) variable. These two allow not only for different effect structures but also for a number of time structures.

For an instantaneous event type intervention variable $I_t^{(1)}$ and a first-order intervention function (9) equation (7) takes the form

$$Y_t^* = (\omega_o - \omega_1)\, I_t^{(1)}.$$

Pior to the event, which is $t < T^{(I)}$, it is that

$$I_i = 0 \text{ and } Y_i^* = \omega_o 0 - \omega_1 0 = 0.$$

At the occurrence of the event at $t = T^{(I)}$ (let $i + 1 = T^{(I)}$)

$$I_{i+1} = 1 \text{ and } Y_{i+1}^* = \omega_o 1 - \omega_1 0 = \omega_o$$

and immediately after for $t = T^{(I)} + 1$

$$I_{i+2} = 0 \text{ and } Y_{i+2}^* = \omega_o 0 - \omega_1 1 = -\omega_1.$$

For $t > T^{(I)} + 1$ we finally obtain (let $i + n = T$)

$$\begin{aligned} I_{i+3} &= 0 \text{ and } Y_{i+3}^* = \omega_o 0 - \omega_1 0 = 0 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= 0 \text{ and } Y_{i+n}^* = \omega_o 0 - \omega_1 0 = 0. \end{aligned}$$

The single event impact $I_t^{(1)}$ in combination with the function (9) produces an effect where a stand-alone pulse ω_o at $T^{(I)}$ is counteracted by another pulse $-\omega_1$ at $T^{(I)} + 1$. Due to the first-order feature of the intervention function the effect immediately dies out after.

Let us now have a temporary event type intervention variable $I_t^{(2)}$ together with function (9), which is in terms of equation (7)

$$Y_t^* = (\omega_o - \omega_1)\, I_t^{(2)}.$$

For $t < T^{(I)}$ without an impact we have

$$I_i = 0 \text{ and } Y_i^* = \omega_o 0 - \omega_1 0 = 0$$

and then, when the event takes place, this is for $T^{(I)} \leq t < T^{(I)} + d$, we observe (let $i + 1 = T^{(I)}$)

$$\begin{aligned} I_{i+1} &= 1 \text{ and } Y_{i+1}^* = \omega_o 1 - \omega_1 0 = \omega_o \\ I_{i+2} &= 1 \qquad Y_{i+2}^* = \omega_o 1 - \omega_1 1 = \omega_o - \omega_1 \\ &\vdots \qquad\qquad \vdots \\ I_{i+m} &= 1 \qquad Y_{i+m}^* = \omega_o 1 - \omega_1 1 = \omega_o - \omega_1. \end{aligned}$$

This is followed by $t = T^{(I)} + d$

$$I_{i+m+1} = 0 \text{ and } Y_{i+m+1}^* = \omega_o 0 - \omega_1 1 = -\omega_1.$$

Afterwards for $t > T^{(I)} + d$ (let $i + n = T$) we have

$$\begin{aligned} I_{i+m+2} &= 0 \text{ and } Y^*_{i+m+2} = \omega_0 0 - \omega_1 0 = 0 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= 0 \qquad Y^*_{i+n} = \omega_0 0 - \omega_1 0 = 0. \end{aligned}$$

The sequence of d event type impacts and the function (9) brings an effect about, which takes its maximum ω_0 at the onset of the intervention and then remains at a level $\omega_0 - \omega_1$ for $d - 1$ time units. The effect ends after a sole countereffect of $-\omega_1$.

For a permanent event type intervention variable and the function (9) we again look at equation (7)

$$Y^*_t = (\omega_0 - \omega_1)\, I_t^{(3)}.$$

Before the event, this is for $t < T^{(I)}$, we have

$$I_i = 0 \text{ and } Y_i^* = \omega_0 0 - \omega_1 0 = 0.$$

With the occurrence of the event for $t \geq T^{(I)}$ (let $i + 1 = T^{(I)}$ and $i + n = T$) we observe

$$\begin{aligned} I_{i+1} &= 1 \text{ and } Y^*_{i+1} = \omega_0 1 - \omega_1 0 = \omega_0 \\ I_{i+2} &= 1 \qquad Y^*_{i+2} = \omega_0 1 - \omega_1 1 = \omega_0 - \omega_1 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= 1 \qquad Y^*_{i+n} = \omega_0 1 - \omega_1 1 = \omega_0 - \omega_1. \end{aligned}$$

This case is related to the above one. We have the same type of intervention effect but permanently remaining at a certain level $\omega_0 - \omega_1$, at least for the period unter investigation.

To pay tribute to even more complex intervention effects we finally consider process type intervention variables for reasons already given.

Let us have a temporary process type intervention variable $I_t^{(4)}$ and again function (9) which yields for equation (7)

$$Y^*_t = (\omega_0 - \omega_1)\, I_t^{(4)}.$$

For $t < T^{(I)}$ prior to the impact process we have

$$I_i = 0 \text{ and } Y_i^* = \omega_0 0 - \omega_1 0 = 0$$

and then during it for $T^{(I)} \leq t < T^{(I)} + d$ (let $i + 1 = T^{(I)}$)

$$\begin{aligned} I_{i+1} &= p_1 \text{ and } Y^*_{i+1} = \omega_0 p_1 = \omega_1 0 = \omega_0 p_1 \\ I_{i+2} &= p_2 \qquad Y^*_{i+2} = \omega_0 p_2 - \omega_1 p_1 \\ &\vdots \qquad\qquad \vdots \\ I_{i+m} &= p_m \qquad Y^*_{i+m} = \omega_0 p_m - \omega_1 p_{m-1}. \end{aligned}$$

For $t = T^{(I)} + d$ $(d = m + 1)$ it is

$$I_{i+m+1} = 0 \text{ and } Y^*_{i+m+1} = \omega_0 0 - \omega_1 p_m = -\omega_1 p_m$$

and in the following for $t > T^{(I)} + d$ (let $i + n = T$)

$$\begin{aligned} I_{i+m+2} &= 0 \text{ and } Y^*_{i+m+2} = \omega_0 0 - \omega_1 0 = 0 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= 0 \qquad Y^*_{i+n} = \omega_0 0 - \omega_1 0 = 0. \end{aligned}$$

For the given series of impacts $I_t^{(4)}$ function (9) can produce an $d + 1$ long effect of a complex shape in dependence of the values p_t and their ordering in time. The dying-out of the intervention effect is preceded by a countereffect which is determined by the very last impact value at $T^{(I)} + d$. As long as we can assume a lag one dependence almost any effect is analysable, given a process input.

The last case we discuss is that of a permanent process type intervention variable in combination with function (9) and equation (7) now being

$$Y_t^* = (\omega_0 - \omega_1)\, I_t^{(5)}.$$

Having $t < T^{(I)}$ without an impact process

$$I_i = 0 \text{ and } Y_1 = \omega_0 0 - \omega_1 0 = 0.$$

For the duration of the impact process, that is for $t \geq T^{(I)}$ we have (let $i + 1 = T^{(I)}$ and $i + n = T$)

$$\begin{aligned} I_{i+1} &= p_1 \text{ and } Y_{i+1} = \omega_0 p_1 - \omega_1 0 = \omega_0 p_1 \\ I_{i+2} &= p_2 \qquad Y_{i+2} = \omega_0 p_2 - \omega_1 p_1 \\ &\vdots \qquad\qquad \vdots \\ I_{i+n} &= p_n \qquad Y_{i+n} = \omega_0 p_n - \omega_1 p_{n-1}. \end{aligned}$$

In this case everything applies which was said for the previous one. The only difference is the fact that the latter accounts for permanent intervention effects, i.e. for the period analysed.

Typical examples for all cases concerning the first-order intervention function are displayed in Figure 2. It can be looked upon as a guide which helps to identify observed intervention effects in dependence of specific inputs and functions.

8. Conclusions

All our considerations are still in the framework of the BOX and TIAO (1975) approach. Chapter 6 and 7 made clear that it is possible and valuable to differentiate between intervention impacts and intervention effects after imposing certain restrictions on the classes of functions under consideration. In practice these restrictions do not bring about any significant reduction in the number of effects which can be analysed. In addition we have seen how diversified the behaviour of the zero- and first-order intervention functions can be, although they only comprise level parameters.

Going back to Table 1 of chapter 4, let us finally discuss which demands are met by our modified BOX and TIAO approach. The fact that we can cope well with the basic demand of discriminating between intervention impacts and intervention effects, enables us to overcome all drawbacks of both the GLASS, WILLSON and GOTTMAN (1975) and the BOX and TIAO (1975) approach.

We are in the position to deal with both event and process type intervention inputs for the class of intervention functions defined. This has been shown and illustrated for a number of zero- and first-order functions. In a further article we will do the same for first- and higher-order intervention functions with level and rate parameters (SCHIMEK, 1988). In addition practical examples will be given and discussed from a statistical point of view.

In general the statistical evaluation of the modified approach is straight forward, as we apply nothing but standard BOX and JENKINS (1976) time series techniques. Due to the fact that a wide variety of observed or chosen (by design) impact series can be analysed, it is in our hands to make use of quasi-experimental designs. If the noise component is known a priori (i.e. a certain ARIMA (p, d, q) process) there is no need for a preintervention series. The intervention model can be estimated without, which is required in many real life evaluations.

Given an intervention series (exogenuous variable) and an observed time series (endogenous variable) in an univariate analysis, existence, effect and time structure can be investigated. This is done by estimating an ordered sequence of models (parameters) with respect to certain intervention functions under a minimum least squares criterion. Because of the linear structure of the intervention models – therefore called linear systems in engineering – additional intervention impacts

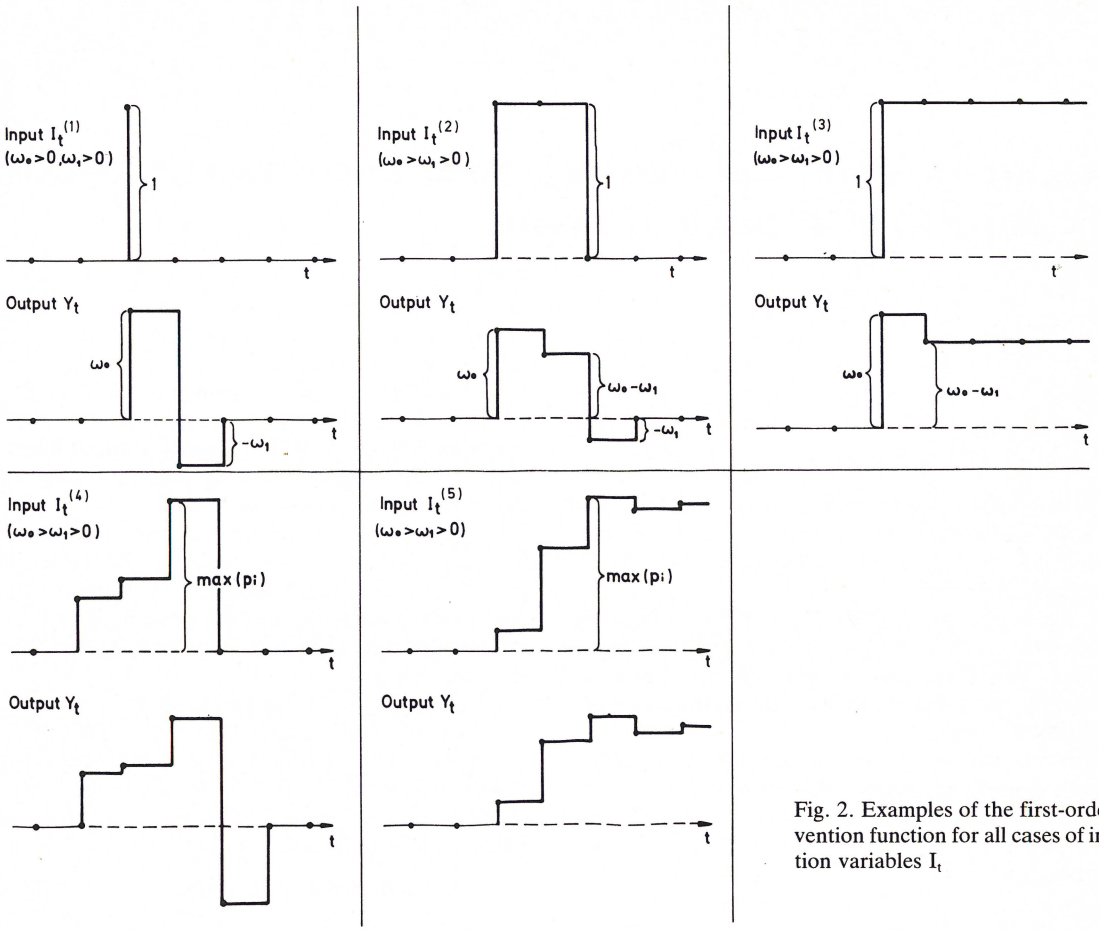

Fig. 2. Examples of the first-order intervention function for all cases of intervention variables I_t

and functions can be added and simultaneously estimated. They allow to study overlapping effects as long as they are linearly decomposable. This makes the approach a powerful tool of an analyst interested in evaluation research. As Table 1 indicates, the modified BOX and TIAO approach meets all the demands defined in chapter 4. Moreover, anyone experienced in BOX and JENKINS time series modelling can easily administer our approach.

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Adresse: Dr. Dr. Michael G. Schimek, Universität Graz, Universitäts-Kinderklinik, Einheit Biometrie, Auenbruggerplatz 30, A-8036 Graz

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The maximum range test – an improved step down procedure for the comparison of all pairs of means

Th. Royen

Summary

Recently a simple step down procedure for the comparison of all pairs of k means based on the maxima of studentized ranges was proposed by ROYEN (1987) including bounds for the multiple level α = 0.05.

*Using bounds of the same table this procedure is improved here by taking into account at each step the **specific** hypotheses rejected before. This procedure is uniformly more powerful than the analogous modified Bonferroni-Holm procedure proposed by SHAFFER (1986).*

Moreover bounds for α = 0.01 are supplied for k = 3 (1) 10 and 42 selected degrees of freedom between 4 and ∞.

Zusammenfassung

Von ROYEN (1987) wurde eine einfache – auf den Maxima studentisierter Spannweiten beruhende – sequentiell ablehnende Testprozedur zum Vergleich aller Paare aus k Mittelwerten vorgeschlagen und eine Tafel mit Schranken zum multiplen Niveau α = 0.05 angegeben.

*Unter Benutzung von Schrankenwerten der gleichen Tafel kann das Verfahren verschärft werden, indem bei jedem Schritt die **spezifischen** zuvor abgelehnten Paarhypothesen berücksichtigt werden. Dieses Verfahren ist gleichmäßig schärfer als die entsprechende modifizierte Bonferroni-Holm-Prozedur nach SHAFFER (1986).*

Darüber hinaus werden Schranken zum Niveau α = 0.01 angegeben für k = 3 (1) 10 und 42 ausgewählte Freiheitsgrade zwischen 4 und ∞.

1. The procedure

The procedure is described for a balanced one-way layout. For an unbalanced layout it is conservative due to a result of HAYTER (1984).

Let be $\bar{y}_1 < \ldots < \bar{y}_k$ the ordered means of k independent samples of equal size n taken from normal distributions with expectations μ_i $(1 \le i \le k)$ and equal variance σ^2. s^2 denotes the usual estimate of σ^2 based on ν degrees of freedom and independent of the means. H_{ij} is the hypothesis $\mu_i = \mu_j$ $(1 \le i < j \le k)$ and $T_{ij} := \sqrt{n}\,|\bar{y}_i - \bar{y}_j|/s$ the corresponding two-sided teststatistic ($|\bar{y}_i - \bar{y}_j|/s\sqrt{(n_i^{-1} + n_j^{-1})/2}$ for the unbalanced case).

Let be $T^K > \ldots > T^1$ $(K := \binom{k}{2})$ the ordered T_{ij} and $H^K, \ldots, H^1$ the corresponding hypotheses. For ties (i.e. several equal T_{ij} values) see end of section 2.

Now a step down procedure operates as follows [1]: beginning with the largest rank r = K the hypothesis H^r is rejected if $T^r \ge c(\alpha, r)$ with a suitable bound $c(\alpha, r)$. If for the first time $T^r < c(\alpha, r)$ is encountered then the procedure ends and $H^r, \ldots, H^1$ are retained. Therefore step r is only reached if $H^K, \ldots, H^{r+1}$ are rejected.

Supposed the specific hypotheses $H^K, \ldots, H^{r+1}$ are wrong, the true H_{ij} are contained in $\mathcal{H}^r := \{H^r, \ldots, H^1\}$. Each configuration of the true $H_{ij} \in \mathcal{H}^r$ corresponds to a »partition« B with disjunct blocks $B_1, \ldots, B_b$ of size ≥2, where each block contains only subscripts of identical μ-values and different blocks belong to distinct μ-values. With each B an intersection or partition hypothesis $H_B = H_{(B_1,\ldots,B_b)} := \bigcap_{l=1}^{b} H_{B_l}$ is associated, wherein $H_{B_l} := \bigcap_{i,j \in B_l} H_{ij}$ (i.e. identical μ_i-values for all $i \in B_l$). Using studentized ranges $Q_l = \max_{i,j \in B_l} T_{ij}$ of blocks B_l the test statistic $Q_B := \max_{1 \le l \le b} Q_l$ (maximal range of B) is associated with H_B. The corresponding nominal level α bounds $q(\alpha, B) = q(\alpha; k_1, \ldots, k_b; \nu)$ depend on B only through the block sizes $k_1, \ldots, k_b$. For the rank r let be $\mathcal{B}^r := \{B \mid Q_B = T^r\}$ and B^r a »least favourable« partition of $\mathcal{B}^r$. This means a partition with a maximal bound $q(\alpha, B)$ in $\mathcal{B}^r$.

Now the proposed test procedure rejects H^r exactly if $H^K, \ldots, H^{r+1}$ are rejected and $T^r \ge c(\alpha, r) := q(\alpha, B^r)$.

For the practical determination of the bounds see section 2 and 3.

The simpler procedure in ROYEN (1987) uses instead of $q(\alpha, B^r)$ the bounds $\max\{q(\alpha; k_1, \ldots, k_b; \nu) \mid \sum_{l=1}^{b} \binom{k_l}{2} \le r\}$. Because $\mathcal{H}^r$ contains at most r true hypotheses given that $H^K, \ldots, H^{r+1}$ are false, the corresponding block sizes k_l satisfy the condition $\sum_{l=1}^{b} \binom{k_l}{2} \le r$ in any case irrespective of the K-r specific hypotheses rejected before, whereas the improved bounds take into account these specific hypotheses.

The refined procedure can be considered also as a closed test procedure. A closed procedure for all intersection hypotheses H_B generated by the minimal hypotheses H_{ij} associates with each H_B a test statistic Z_B and a nominal level α bound $c(\alpha, B)$. To ensure the coherence of the procedure, H_B is rejected exactly if $Z_{B'} \ge c(\alpha, B')$ for all $H_{B'}$ implying H_B (B included). Such procedures ensure the multiple level α (or type I familywise error rate α, briefly FWE) (see HOCHBERG & TAMHANE, 1987).

[1] Users may also directly look at the examples given in section 2.

The following two additional requirements seem to be reasonable:
Requirement 1: the tests associated with the H_B should exhaust the nominal level α, i.e. $P\{Z_B \geq c(\alpha, B) \mid H_B \text{ true}\} = \alpha$. This is not satisfied by the known*) more step procedures for pair comparisons based on ranges and keeping the type I FWE α (see HOCHBERG & TAMHANE, 1987).
Requirement 2: a difference of means should never be rejected if a larger one is retained. Otherwise users will hardly accept the procedure. This seems to be a natural demand if the minimal hypotheses H_{ij} are of primary interest and not the whole set of homogeneity hypotheses for all subsets of $\{\mu_1 \ldots, \mu_k\}$ of size ≥ 2, which generate the same set of intersection hypotheses H_B.

Obviously the test procedure given above satisfies these two requirements. Conversely, if a closed procedure using the test statistics Q_B for the H_B rejects a H_B then it must reject $H_{B'}$ for all $H_{B'}$ implying H_B. For the B' with $Q_{B'} = T^r = Q_B$ this enforces the bound $\max\{q(\alpha, B') \mid B' \in \mathscr{B}^r\}$ for T^r and requirement 2 entails the step down performance of the single tests.

Instead of the tabulated bounds the tail probabilities $p(T_{ij} \mid B) :=$ probability that the random variable Q_B exceeds the observed value T_{ij} given that H_B is true may be used. At step r, H^r is rejected exactly if $\max\{p(T_{ij} \mid B) \mid B \in \mathscr{B}^r\} \leq \alpha$.

2. Examples

The search for the required bound at step r is explained by an example with k = 8 means. A simple algorithm for the single steps of the procedure is given in section 3.

The notation $[i, j] := \{i, i+1, \ldots, j\}$ is used for a block of size $k = j - i + 1$ with the »endpoints« i, j. $\mathscr{H}^r$ means here the set of pairs (i, j) belonging to the non rejected H_{ij} (i.e. belonging to the differences of rank $\leq r$) at the beginning of step r. Let be $r = 10$, $T^{10} = T_{i_o,j_o} = T_{1,2}$ and $\mathscr{H}^r = \{(1,2), (2,3), (3,4), (4,5), (5,6), (6,7), (7,8), (4,6), (5,7), (6,8)\}$.

All pairs having an element in common with $[i_o, j_o]$ (here [1,2]) are cancelled which gives the reduced set $\mathscr{H}_o^{1o} = \{(3,4), \ldots, (6,8)\}$. A partition $[i_o, j_o], [i_1, j_1], \ldots$ of disjunct blocks with their pairs of endpoints (i_l, j_l) in $\mathscr{H}^{1o}$ and block sizes $k_o, k_1, \ldots$ giving a maximal bound $q(\alpha; k_o, k_1, \ldots; \nu) = c(\alpha, 10)$ has to be found. The restriction to non-overlapping blocks $[i_l, j_l]$ is explained in section 3.

For simplicity the sizes $(k_o, k_1, \ldots)$ are called also a »partition«. A look at table 1 shows that for the rank $r = 10$ the uppermost partition (irrespective of the H_{ij} rejected before) is given by a single block of size 5. If the rank r is not contained in table 1 the partition belonging to the next upper tabulated rank has to be taken. The partitions in table 2 which must be examined are below this partition (5) and they must contain the number 2 because $[i_o, j_o] = [1,2]$ is of size 2. Subject to the conditions $\sum_1 k_l \leq k = 8$, $\sum_1 \binom{k_l}{2} \leq r = 10$ these are the partitions (4,2,2), (3,3,2), (4,2), (3,2,2), (2,2,2,2), ... Because H_o^{10} does not contain endpoints of a block of size 4 the partition (3,3,2) is the next candidate to be checked. The only partition of this type would be [1,2], [3,5], [6,8], but it is not admissible because (3,5) does not belong to H_o^{10}. The next possible size partition (3,2,2) is the right one because e.g. [1,2], [3,4], [5,7] or [1,2], [4,5], [6,8] are of this type. The corresponding bound for $T_{1,2} = T^{10}$ with $\alpha = 0.01$ and $\nu = 40$ e.g. is given by $q(0.01; 3,2,2; 40) = 4.649$.

The simpler procedure in ROYEN (1987) gives only the bound $q(0.01; 5; 40) = 4.931$.

If there are some means between $\bar{y}_{i_o}, \bar{y}_{j_o}$ the search is more complicated because it is not generally allowed only to take the full block $[i_o, j_o]$ of size $j_o - i_o + 1$ into consideration. Every subset with the endpoints i_o, j_o must be considered as a possible block with the range $\bar{y}_{j_o} - \bar{y}_{i_o}$. This is taken into account by the algorithm in section 3.

Especially for $\binom{k}{2} > r \geq \binom{k-1}{2}$ the simpler procedure applies the constant bound $q(\alpha; k-1; \nu)$. The improvement for these ranks is illustrated by the following example with $k = 6$, $n = 5$, $\nu = 4 \cdot 6 = 24$, $\bar{y}_1 = 10$, $\bar{y}_2 = 11$, $\bar{y}_3 = 11.95$, $\bar{y}_4 = 12.05$, $\bar{y}_5 = 16.1$, $\bar{y}_6 = 17$ and $s = \sqrt{5}$:

The simpler procedure rejects only $H_{1,6}$, $H_{1,5}$ and $H_{2,6}$ because the bound 5.168 is used down to the rank $r = 10$. Note that the bounds depending on the previous rejections not necessarily decline from step to step.

If there are ties among the T_{ij} a random assignment of the ranks belonging to the tied group is possible but this can entail different decisions over the significance of equal differences. It is also possible to determine all partitions $(k_1, k_2, \ldots)$ for the ranks of a tied group according to the algorithm described in the following section and then to use the largest bound belonging to these partitions for all the identical differences of this group.

Rank	(i, j)	$T_{ij} = \lvert\bar{y}_i - \bar{y}_j\rvert$	partition	0.01-bound	significance	
15	1,6	7.0	6	5.374	*	
14	1,5	6.1	5	5.168	*	
13	2,6	6.0	5	5.168	*	
12	2,5	5.1	4	4.907	*	
11	3,6	5.05	4,2	5.010	*	
10	4,6	4.95	3,3	4.948	*	
9	3,5	4.15	3,2	4.727	–	end of procedure

3. An algorithm for the single step

For r with $T^r = T_{i_o j_o}$ the correct bound $c(\alpha, r)$ has to be found. For this search only partitions $K = (k_1, \ldots, k_b)$ of block sizes satisfying the conditions $\sum_1 k_l \leq k$ and $\sum_1 \binom{k_l}{2} \leq r$ are admissible. These K are ordered according to the values of the corresponding level α bounds. This order may depend also on ν, especially for small ν. The highest admissible $K = K^r$ is taken from table 1. Beginning with $K = K^r$ the admissible partitions K are examined downwards if there exists a block partition with all its pairs of endpoints (i_l, j_l) in $\mathscr{H}^r$ $(0 \leq l \leq b-1)$ and having the same block sizes like K (apart from the order). The highest K satisfying these requirements gives the desired bound $c(\alpha, r) = q(\alpha; K; \nu)$.

For k_o: $= j_o - i_o + 1 \geq k - 2$ no algorithm is needed. The bound is $q(\alpha; k_o; \nu)$ for $k_o \geq k - 1$. For $k_o = k - 2$ there are the

*) A program using a different algorithm for the closed maximum range test without requirement 2 was already presented by H. Finner (University of Trier). This program compares up to 20 means. Finner's algorithm was not submitted for publication until the writing of the present paper.
See H. Finner: »Der abgeschlossene Newman-Keuls Test«, lecture, held on the 32th Colloquium of the German Section of the Biometric Society in Ulm, march 18–21, 1986. (Personal communication of H. Finner.)

following cases: The two means outside the interval $[\bar{y}_{i_o}, \bar{y}_{j_o}]$ are separated by the interval or they are on the same side of this interval but the rank of their absolut difference is larger then r. Then $q(\alpha; k_o; \nu)$ is the correct bound. Otherwise $q(\alpha; k_o, 2; \nu)$ has to be taken. Therefore in any case the least favourable partition contains the full block $[i_o, j_o] = \{i_o, i_o + 1, \ldots, j_o\}$. This is not generally valid for $j_o - i_o + 1 \leq k - 3$.

Now for simplicity the means belonging to the subscripts of a block are also called a block. If $\bar{y}_{j_o} - \bar{y}_{i_o}$ is the range of a block of unknown size $k_o \geq 2$ any further means of this block must be located between $\bar{y}_{i_o}$ and $\bar{y}_{j_o}$. For any fix choice B'_o of the $2^{j_o - i_o - 1}$ possible subsets of $\{i_o + 1, i_o + 2, \ldots, j_o - 1\}$ the reduced set $\mathscr{H}^r_o$ of the remaining pairs is defined by $\{(i, j) \in \mathscr{H}^r \mid i, j \notin B_o := B'_o \cup \{i_o, j_o\}\}$.

Any further blocks B_l $(l > 0)$ with ranges $\bar{y}_{j_l} - \bar{y}_{i_l}$ may overlap but at the end of this section the restriction to non overlapping blocks is justified. By this restriction the algorithm is simplified to a search in comparatively small trees. If all the remaining numbers in $\mathscr{H}^r_o$ are renumbered from 1 to h_o then the block $[i_l, j_l]$ $(l > 0)$ has the size $j_l - i_l + 1$.

If a partition K matches a block partition $B = (B_o, [i_1, j_1], \ldots, [i_{b-1}, j_{b-1}])$ then the size k_o of B_o must occur in K. Cancelling k_o from K gives the reduced partition K_o with the renumbered sizes $k_1 \geq .. \geq k_{b-1}$. These sizes must coincide with the numbers $j_l - i_l + 1$ in some order. The search for a block partition matching a given K corresponds to a path upwards in a tree wherein the nodes of level l correspond to the pairs (i_l, j_l) $(0 \leq l \leq b - 1)$. The root of this tree is given by $N_o := ((i_o, j_o), \mathscr{H}(N_o) := \mathscr{H}^r_o)$. Generally a node is characterized by a pair (i, j), the set $\mathscr{H}(N)$ of the remaining pairs and its level l. N' is a successor of N exactly if it has the level $l' = l + 1$ and a characteristic pair $(i', j') \in \mathscr{H}(N)$ with the size $j' - i' + 1 = k_{l+1}$. Then $\mathscr{H}(N')$ equals $\{(i, j) \in \mathscr{H}(N) \mid i, j \notin [i', j']\}$.

The search is repeated for all possible subsets B'_o because the tree depends on the choice of B'_o. If for the first time a node of level $b - 1$ bas been found then the just examined K gives the required bound $c(\alpha, r)$. The following structogram may facilitate the coding of this algorithm[2].

The restriction to non overlapping blocks is based on the following inequality for the distribution functions F_k of the ranges of k independent identical distributed normal random variables:

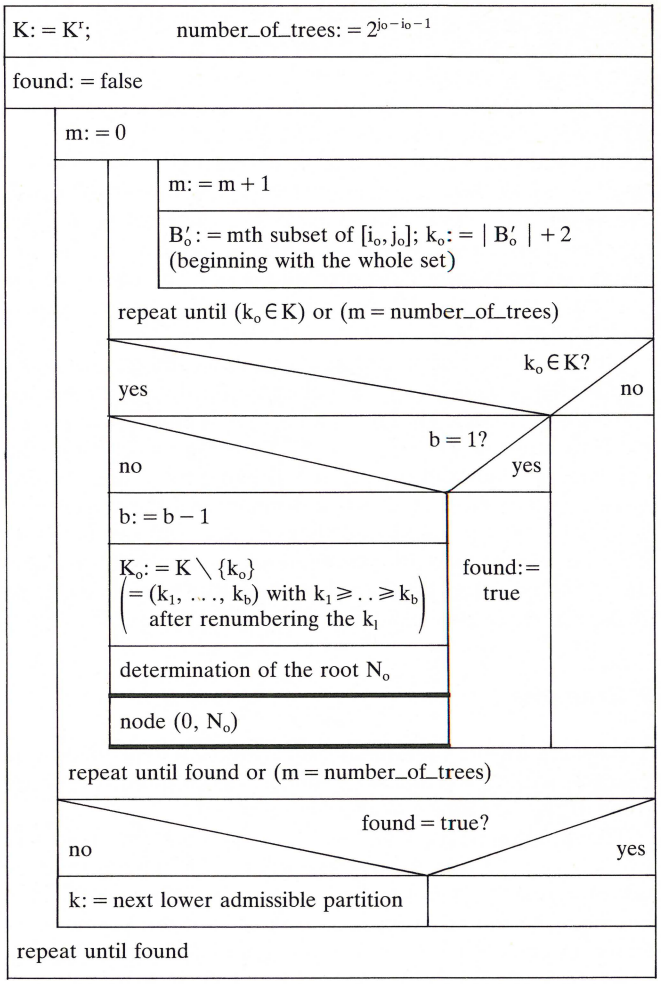
$$F_{k_1}(x) \cdot F_{k_2}(x) - F_{k_1+1}(x) \cdot F_{k_2-1}(x) > 0$$
for all integers $k_1 \geq k_2 \geq 2$ and all $x > 0$.
$(F_1(x) = 1$ for all $x > 0)$

The mathematical proof is given in a different paper. For the testprocedure only the resulting inequality for the corresponding level α bounds is really needed which can be verified directly by inspection of the tables. Obviously the inequality must also be valid for studentized ranges.

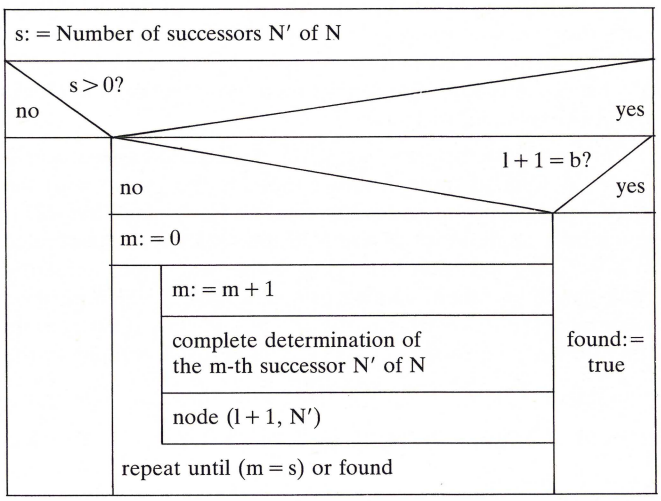
Now let be B_1, B_2 two overlapping blocks of means with sizes $k_1 \geq k_2$ and ranges $Q_{k_1} = \bar{y}_{j_1} - \bar{y}_{i_1}$ and Q_{k_2}. If all means of B_2 between $\bar{y}_{i_1}$ and $\bar{y}_{j_1}$ are transferred to B_1 then $\max(Q_{k_1}, Q_{k_2})$ is stochastically increased according to the inequality given above. Therefore the overlapping blocks of any admissible block partition may be separated step by step giving admissible block partitions B again with increased level α bounds for the maximal range Q_B. Only the root block B_o is not included in this process because its endpoints $\bar{y}_{i_o}$, $\bar{y}_{j_o}$ must be kept fixed.

[2] The algorithm can be refined at the cost of greater complexity.

Procedure step (only needed for $k > 5$, $j_o - i_o - 1 \leq k - 5$)



Procedure node (l, N)



4. Tables

The rows of table 2 are ordered according to the values of the bounds for the degree of freedom $\nu = \infty$. To save some interpolations, all $\nu \leq 60$ not containing primes ≥ 11 are included because ν is frequently a product of small numbers in balanced Anova designs.

Table 1 (for level $\alpha = 0.01$)

k = 3

rank	partition
3	3
2	2

4

rank	partition
6	4
5	3
2	2,2
1	2

5

rank	partition
10	5
9	4
5	3,2
3	3
2	2,2
1	2

6

rank	partition
15	6
14	5
9	4,2
6	3,3
5	3,2
3	2,2,2
2	2,2
1	2

10

rank	partition
45	10
44	9
35	8,2
28	8
27	7,3
23	7,2 $\nu \geq 56$
21	6,4
20	5,5
19	6,3
17	6,2,2 $\nu \geq 5$
16	5,4
15	6 $\nu \geq 56$
14	5,3,2
13	4,4,2
12	4,3,3
11	5,2 $\nu \geq 12$
10	4,3,2
9	3,3,3
8	3,3,2,2
7	3,3,2
6	3,2,2,2
5	2,2,2,2,2
4	2,2,2,2
3	2,2,2
2	2,2
1	2

9

rank	partition
36	9
35	8
27	7,2
21	7
20	6,3
17	5,4
15	6 $\nu \geq 5$
14	5,3
12	4,4
11	5,2 $\nu \geq 12$
10	4,3,2
9	3,3,3
8	4,2,2
7	3,3,2
6	3,2,2,2
5	3,2,2
4	2,2,2,2
3	2,2,2
2	2,2
1	2

8

rank	partition
28	8
27	7
20	6,2
15	6 $\nu \geq 5$
14	5,3
12	4,4
11	5,2
10	5 $\nu \geq 12$
9	4,3
8	4,2,2
7	3,3,2
6	3,3
5	3,2,2
4	2,2,2,2
3	2,2,2
2	2,2
1	2

7

rank	partition
21	7
20	6
14	5,2
10	5 $\nu \geq 12$
9	4,3
8	4,2
6	3,3
5	3,2,2
4	3,2
3	2,2,2
2	2,2
1	2

For degrees of freedom below the indicated values the partition of the next line has to be taken. (For $k \leq 6$ the table is also valid for $\alpha = 0.05$)

Table 2 (Level Alpha = 0.01)

DG of freedom:	4	5	6	7	8	9	10
Partition:							
10:	12.265	10.239	9.097	8.368	7.863	7.495	7.213
9:	11.925	9.972	8.869	8.166	7.681	7.325	7.055
82:	11.667	9.762	8.688	8.004	7.530	7.185	6.921
8:	11.542	9.669	8.613	7.939	7.474	7.134	6.875
73:	11.483	9.611	8.555	7.882	7.418	7.078	6.820
72:	11.258	9.439	8.413	7.760	7.308	6.979	6.728
64:	11.371	9.518	8.473	7.807	7.348	7.012	6.756
55:	11.334	9.487	8.446	7.782	7.324	6.989	6.734
7:	11.101	9.321	8.318	7.679	7.237	6.915	6.669
63:	11.068	9.282	8.275	7.634	7.191	6.868	6.622
622:	10.969	9.203	8.208	7.575	7.138	6.818	6.575
54:	10.972	9.202	8.204	7.569	7.130	6.810	6.567
62:	10.788	9.066	8.097	7.479	7.053	6.742	6.505
6:	10.583	8.913	7.973	7.373	6.960	6.658	6.428
532:	10.794	9.058	8.081	7.458	7.029	6.715	6.476
442:	10.735	9.009	8.037	7.418	6.991	6.679	6.442
53:	10.597	8.909	7.958	7.352	6.935	6.630	6.398
433:	10.656	8.944	7.980	7.366	6.942	6.633	6.398
44:	10.533	8.855	7.910	7.309	6.894	6.591	6.360
522:	10.474	8.810	7.873	7.277	6.866	6.566	6.338

DG of freedom:	4	5	6	7	8	9	10
Partition:							
52:	10.235	8.630	7.726	7.150	6.753	6.464	6.243
432:	10.314	8.677	7.756	7.170	6.766	6.471	6.246
5:	9.958	8.421	7.556	7.005	6.625	6.348	6.136
333:	10.219	8.598	7.686	7.106	6.706	6.414	6.192
4222:	10.175	8.565	7.659	7.083	6.685	6.396	6.175
43:	10.058	8.482	7.595	7.031	6.642	6.358	6.142
3322:	10.074	8.481	7.584	7.014	6.622	6.335	6.117
422:	9.899	8.354	7.485	6.932	6.551	6.273	6.061
332:	9.784	8.259	7.400	6.854	6.478	6.204	5.995
42:	9.572	8.106	7.280	6.755	6.393	6.129	5.928
3222:	9.606	8.113	7.274	6.740	6.373	6.104	5.901
33:	9.440	7.995	7.182	6.665	6.309	6.049	5.851
4:	9.173	7.804	7.033	6.543	6.204	5.957	5.769
22222:	9.413	7.955	7.136	6.615	6.256	5.995	5.796
322:	9.229	7.823	7.033	6.530	6.184	5.931	5.739
2222:	8.998	7.633	6.866	6.379	6.043	5.798	5.612
32:	8.755	7.460	6.731	6.268	5.948	5.715	5.538
222:	8.465	7.220	6.521	6.076	5.769	5.546	5.376
3:	8.120	6.976	6.331	5.919	5.635	5.428	5.270
22:	7.724	6.647	6.040	5.654	5.387	5.192	5.044
2:	6.512	5.702	5.243	4.949	4.746	4.596	4.482

Table 2 (Level Alpha = 0.01)

DG of freedom:	12	14	15	16	18	20	21
Partition:							
10:	6.814	6.543	6.439	6.349	6.201	6.087	6.038
9:	6.670	6.409	6.309	6.222	6.081	5.970	5.924
82:	6.547	6.294	6.197	6.112	5.975	5.868	5.823
8:	6.507	6.258	6.162	6.079	5.944	5.839	5.794
73:	6.453	6.205	6.109	6.026	5.892	5.787	5.743
72:	6.371	6.131	6.038	5.958	5.827	5.725	5.682
64:	6.393	6.148	6.053	5.971	5.838	5.734	5.691
55:	6.372	6.128	6.033	5.952	5.820	5.716	5.673
7:	6.321	6.085	5.994	5.915	5.788	5.688	5.646
63:	6.273	6.037	5.946	5.868	5.740	5.640	5.598
622:	6.230	5.998	5.908	5.830	5.704	5.606	5.565
54:	6.221	5.987	5.897	5.819	5.693	5.594	5.553
62:	6.169	5.942	5.854	5.779	5.656	5.560	5.519
6:	6.101	5.881	5.796	5.722	5.603	5.510	5.470
532:	6.138	5.910	5.821	5.746	5.622	5.526	5.485
442:	6.106	5.879	5.791	5.716	5.593	5.497	5.457
53:	6.069	5.847	5.761	5.687	5.567	5.473	5.433
433:	6.065	5.840	5.753	5.678	5.557	5.462	5.422
44:	6.033	5.813	5.727	5.654	5.535	5.442	5.402
522:	6.014	5.795	5.711	5.638	5.520	5.428	5.389
52:	5.931	5.720	5.638	5.568	5.454	5.365	5.327
432:	5.928	5.714	5.631	5.560	5.444	5.353	5.315
5:	5.836	5.634	5.556	5.489	5.379	5.294	5.257
333:	5.878	5.666	5.584	5.513	5.398	5.309	5.271
4222:	5.863	5.653	5.571	5.501	5.387	5.299	5.261
43:	5.835	5.629	5.549	5.480	5.369	5.281	5.245
3322:	5.808	5.600	5.520	5.451	5.338	5.251	5.214
422:	5.761	5.559	5.481	5.414	5.305	5.220	5.184
332:	5.699	5.500	5.423	5.357	5.249	5.165	5.130
42:	5.643	5.451	5.377	5.313	5.209	5.128	5.094
3222:	5.612	5.417	5.342	5.278	5.173	5.091	5.056
33:	5.571	5.382	5.309	5.246	5.144	5.064	5.031
4:	5.502	5.322	5.252	5.192	5.094	5.018	4.986
22222:	5.515	5.325	5.252	5.189	5.087	5.007	4.973
322:	5.467	5.284	5.213	5.152	5.053	4.976	4.943
2222:	5.349	5.171	5.103	5.044	4.948	4.873	4.842
32:	5.286	5.117	5.051	4.995	4.903	4.832	4.801
222:	5.135	4.973	4.910	4.856	4.768	4.700	4.671
3:	5.046	4.895	4.836	4.786	4.703	4.639	4.612
22:	4.834	4.692	4.637	4.590	4.513	4.453	4.428
2:	4.320	4.210	4.168	4.131	4.071	4.024	4.004

DG of freedom:	24	25	27	28	30	32	35
Partition:							
10:	5.919	5.886	5.828	5.802	5.756	5.716	5.666
9:	5.809	5.778	5.722	5.697	5.653	5.615	5.566
82:	5.712	5.681	5.627	5.603	5.560	5.523	5.476
8:	5.685	5.655	5.602	5.578	5.536	5.500	5.453
73:	5.634	5.604	5.551	5.528	5.486	5.449	5.403
72:	5.577	5.547	4.496	5.473	5.433	5.398	5.353
64:	5.583	5.553	5.501	5.478	5.437	5.401	5.355
55:	5.565	5.536	5.484	5.461	5.420	5.384	5.339
7:	5.542	5.513	5.463	5.441	5.401	5.367	5.323
63:	5.495	5.466	5.416	5.394	5.354	5.320	5.276
622:	5.463	5.434	5.385	5.363	5.324	5.290	5.247
54:	5.450	5.422	5.372	5.350	5.311	5.277	5.234
62:	5.420	5.393	5.344	5.323	5.285	5.251	5.209
6:	5.374	5.347	5.300	5.279	5.242	5.210	5.169
532:	5.385	5.357	5.309	5.287	5.249	5.216	5.174

DG of freedom:	24	25	27	28	30	32	35
Partition:							
442:	5.357	5.330	5.282	5.260	5.222	5.189	5.147
53:	5.336	5.309	5.262	5.241	5.204	5.171	5.130
433:	5.324	5.296	5.249	5.228	5.190	5.157	5.116
44:	5.306	5.279	5.232	5.212	5.175	5.142	5.102
522:	5.293	5.267	5.221	5.200	5.164	5.132	5.091
52:	5.235	5.209	5.164	5.144	5.109	5.078	5.039
432:	5.221	5.195	5.150	5.130	5.094	5.063	5.023
5:	5.168	5.144	5.101	5.082	5.048	5.018	4.980
333:	5.179	5.153	5.108	5.088	5.053	5.022	4.983
4222:	5.169	5.144	5.099	5.080	5.044	5.014	4.975
43:	5.154	5.129	5.085	5.066	5.031	5.001	4.963
33222:	5.123	5.098	5.054	5.034	5.000	4.969	4.931
422:	5.095	5.071	5.028	5.009	4.975	4.946	4.909
332:	5.043	5.019	4.976	4.958	4.924	4.895	4.859
42:	5.010	4.986	4.945	4.927	4.895	4.867	4.832
3222:	4.971	4.948	4.907	4.889	4.856	4.828	4.792
33:	4.948	4.925	4.885	4.867	4.836	4.808	4.773
4:	4.907	4.885	4.847	4.830	4.799	4.773	4.739
22222:	4.891	4.868	4.828	4.810	4.779	4.751	4.716
322:	4.863	4.841	4.802	4.785	4.754	4.727	4.694
2222:	4.764	4.743	4.705	4.689	4.659	4.634	4.601
32:	4.727	4.707	4.671	4.655	4.626	4.602	4.570
222:	4.600	4.581	4.546	4.531	4.504	4.480	4.450
3:	4.546	4.527	4.495	4.481	4.455	4.433	4.404
22:	4.366	4.348	4.318	4.305	4.281	4.260	4.234
2:	3.956	3.942	3.918	3.908	3.889	3.873	3.852

DG of freedom:	36	40	42	45	48	49	50
Partition:							
10:	5.651	5.599	5.577	5.548	5.522	5.514	5.507
9:	5.552	5.502	5.481	5.453	5.428	5.421	5.414
82:	5.462	5.414	5.394	5.366	5.343	5.335	5.329
8:	5.439	5.392	5.372	5.345	5.322	5.315	5.308
73:	5.390	5.343	5.322	5.296	5.273	5.266	5.259
72:	5.340	5.294	5.274	5.248	5.226	5.219	5.213
64:	5.342	5.295	5.276	5.249	5.226	5.219	5.213
55:	5.325	5.279	5.259	5.233	5.210	5.203	5.197
7:	5.310	5.265	5.246	5.220	5.198	5.192	5.185
63:	5.263	5.218	5.199	5.174	5.152	5.145	5.139
622:	5.234	5.190	5.171	5.146	5.125	5.118	5.112
54:	5.221	5.177	5.158	5.133	5.111	5.105	5.098
62:	5.197	5.154	5.135	5.111	5.090	5.084	5.077
6:	5.156	5.114	5.097	5.073	5.052	5.046	5.040
532:	5.161	5.118	5.100	5.075	5.054	5.048	5.041
442:	5.135	5.092	5.074	5.050	5.029	5.022	5.016
53:	5.118	5.076	5.058	5.034	5.014	5.007	5.001
433:	5.103	5.061	5.043	5.019	4.998	4.992	4.986
44:	5.090	5.048	5.030	5.007	4.986	4.980	4.974
522:	5.079	5.038	5.020	4.997	4.977	4.971	4.965
52:	5.028	4.988	4.971	4.948	4.928	4.922	4.917
432:	5.011	4.971	4.954	4.931	4.911	4.905	4.899
5:	4.969	4.931	4.914	4.893	4.874	4.868	4.863
333:	4.971	4.931	4.914	4.892	4.872	4.866	4.860
4222:	4.964	4.924	4.907	4.885	4.865	4.859	4.854
43:	4.952	4.913	4.896	4.874	4.855	4.849	4.843
3322:	4.920	4.881	4.864	4.842	4.823	4.817	4.811
422:	4.898	4.860	4.843	4.822	4.803	4.797	4.792
332:	4.848	4.810	4.794	4.773	4.755	4.749	4.744
42:	4.821	4.785	4.769	4.749	4.731	4.725	4.720

Table 2 (Level Alpha = 0.01)

DG of freedom:	36	40	42	45	48	49	50
Partition:							
3222:	4.781	4.745	4.729	4.709	4.691	4.685	4.680
33:	4.763	4.727	4.712	4.692	4.674	4.669	4.664
4:	4.729	4.696	4.681	4.661	4.644	4.639	4.634
22222:	4.706	4.670	4.655	4.635	4.618	4.613	4.607
322:	4.684	4.649	4.634	4.615	4.598	4.593	4.588
2222:	4.591	4.558	4.544	4.525	4.508	4.503	4.499
32:	4.561	4.529	4.515	4.497	4.481	4.476	4.472
222:	4.441	4.410	4.397	4.380	4.365	4.360	4.356
3:	4.396	4.367	4.355	4.339	4.324	4.320	4.316
22:	4.226	4.199	4.187	4.172	4.159	4.155	4.151
2:	3.846	3.825	3.816	3.804	3.793	3.790	3.787

DG of freedom:	54	56	60	65	70	75	80
Partition:							
10:	5.480	5.468	5.447	5.424	5.404	5.387	5.372
9:	5.388	5.376	5.356	5.334	5.315	5.299	5.284
82:	5.304	5.292	5.273	5.251	5.233	5.217	5.203
8:	5.283	5.272	5.253	5.231	5.214	5.198	5.185
73:	5.234	5.224	5.204	5.183	5.165	5.150	5.137
72:	5.189	5.178	5.159	5.139	5.122	5.107	5.094
64:	5.189	5.178	5.159	5.138	5.121	5.105	5.092
55:	5.173	5.162	5.143	5.122	5.105	5.090	5.076
7:	5.162	5.152	5.133	5.113	5.096	5.081	5.069
63:	5.116	5.105	5.087	5.067	5.050	5.036	5.023
622:	5.089	5.079	5.060	5.041	5.024	5.010	4.997
54:	5.075	5.065	5.047	5.027	5.011	4.996	4.984
62:	5.055	5.045	5.027	5.008	4.992	4.978	4.966
6:	5.018	5.009	4.991	4.973	4.957	4.943	4.931
532:	5.019	5.009	4.991	4.972	4.956	4.942	4.930
442:	4.994	4.984	4.966	4.947	4.931	4.917	4.905
53:	4.980	4.970	4.953	4.934	4.918	4.904	4.892
433:	4.964	4.954	4.937	4.918	4.902	4.888	4.876
44:	4.952	4.943	4.925	4.907	4.891	4.878	4.866
522:	4.943	4.934	4.917	4.899	4.883	4.869	4.858
52:	4.896	4.887	4.870	4.853	4.837	4.824	4.813
432:	4.878	4.869	4.852	4.834	4.819	4.806	4.794
5:	4.843	4.834	4.818	4.801	4.786	4.774	4.763
333:	4.840	4.830	4.814	4.796	4.781	4.768	4.757
4222:	4.833	4.824	4.808	4.790	4.775	4.762	4.751
43:	4.823	4.814	4.798	4.781	4.766	4.753	4.742
3322:	4.791	4.782	4.766	4.748	4.734	4.721	4.710
422:	4.772	4.763	4.748	4.731	4.716	4.704	4.693
332:	4.724	4.715	4.700	4.683	4.669	4.657	4.646
42:	4.701	4.693	4.678	4.662	4.648	4.636	4.626
3222:	4.661	4.653	4.637	4.621	4.608	4.596	4.585
33:	4.645	4.637	4.622	4.606	4.593	4.581	4.571
4:	4.617	4.609	4.595	4.579	4.566	4.555	4.545
22222:	4.589	4.581	4.566	4.550	4.537	4.525	4.515
322:	4.570	4.562	4.547	4.532	4.519	4.508	4.498
2222:	4.481	4.474	4.460	4.445	4.432	4.422	4.412
32:	4.455	4.448	4.434	4.420	4.408	4.397	4.388
222:	4.340	4.333	4.320	4.307	4.295	4.285	4.277
3:	4.301	4.294	4.282	4.269	4.258	4.249	4.241
22:	4.137	4.131	4.120	4.108	4.097	4.089	4.081
2:	3.776	3.771	3.762	3.753	3.745	3.738	3.732

DG of freedom:	90	100	120	150	200	300	∞
Partition:							
10:	5.348	5.328	5.299	5.270	5.242	5.213	5.157
9:	5.261	5.242	5.214	5.187	5.159	5.132	5.078
82:	5.181	5.163	5.136	5.109	5.082	5.056	5.003
8:	5.162	5.144	5.118	5.091	5.065	5.039	4.987
73:	5.114	5.097	5.070	5.044	5.018	4.992	4.941
72:	5.072	5.055	5.029	5.004	4.979	4.953	4.904
64:	5.070	5.053	5.027	5.001	4.975	4.950	4.899
55:	5.055	5.037	5.011	4.986	4.960	4.935	4.885
7:	5.048	5.031	5.005	4.980	4.956	4.931	4.882
63:	5.002	4.985	4.960	4.935	4.911	4.886	4.838
622:	4.977	4.960	4.935	4.911	4.887	4.862	4.815
54:	4.963	4.946	4.922	4.897	4.873	4.848	4.801
62:	4.945	4.929	4.905	4.881	4.857	4.834	4.787
6:	4.911	4.896	4.872	4.849	4.826	4.803	4.757
532:	4.909	4.893	4.869	4.845	4.821	4.798	4.751
442:	4.885	4.869	4.845	4.821	4.798	4.774	4.728
53:	4.873	4.857	4.833	4.810	4.787	4.764	4.718
433:	4.856	4.840	4.816	4.793	4.770	4.746	4.701
44:	4.846	4.830	4.807	4.784	4.761	4.738	4.693
522:	4.838	4.823	4.800	4.777	4.754	4.732	4.687
52:	4.794	4.779	4.757	4.735	4.713	4.691	4.647
432:	4.775	4.760	4.737	4.715	4.693	4.671	4.627
5:	4.745	4.730	4.709	4.687	4.666	4.645	4.603
333:	4.738	4.723	4.701	4.679	4.657	4.635	4.592
4222:	4.732	4.717	4.695	4.673	4.651	4.630	4.587
43:	4.724	4.709	4.687	4.666	4.644	4.623	4.581
3322:	4.691	4.677	4.655	4.633	4.612	4.590	4.548
422:	4.675	4.661	4.640	4.618	4.597	4.576	4.535
332:	4.629	4.615	4.594	4.573	4.552	4.532	4.491
42:	4.609	4.595	4.575	4.554	4.534	4.514	4.475
3222:	4.568	4.554	4.534	4.514	4.494	4.474	4.434
33:	4.554	4.541	4.521	4.501	4.481	4.462	4.423
4:	4.529	4.516	4.497	4.478	4.459	4.440	4.403
22222:	4.499	4.485	4.466	4.446	4.426	4.407	4.369
322:	4.482	4.469	4.450	4.430	4.411	4.392	4.355
2222:	4.396	4.384	4.365	4.347	4.328	4.310	4.274
32:	4.373	4.361	4.343	4.325	4.308	4.290	4.255
222:	4.262	4.251	4.234	4.216	4.200	4.183	4.150
3:	4.227	4.216	4.200	4.184	4.168	4.152	4.120
22:	4.068	4.058	4.043	4.028	4.013	3.998	3.969
2:	3.722	3.714	3.702	3.690	3.678	3.666	3.643

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Address of the author: Prof. Dr. Th. Royen, Fachhochschule Rheinland-Pfalz, Abteilung Bingen, Rochusallee 4, D-6530 Bingen

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Transformation of data and identification of outliers – as experienced in an epidemiological study

A. Bartkowiak, S. Lukasik, K. Chwistecki, M. Mrukowicz, W. Morgenstern

Summary

This paper is a continuation of our former work (BARTKOWIAK et al., 1987).

Formerly we have identified some outliers in some epidemiological data comprising observations in seven coronary heart disease risk variables. We did it using mainly Mahalanobis distances and the first two and last two principal components.

Now we have been interested in the following problem: what happens, when the data are transformed (simply rescaled or transformed by the Box-Cox formula)? Do we find the same outliers?

We have found, that the principal components, evaluated from the transformed data, can be entirely different. None the less, the mostly gross outliers could be identified.

Zusammenfassung

Diese Arbeit ist eine Fortsetzung von unserer früheren Veröffentlichung (BARTKOWIAK et al., 1987).

Es handelte sich um ein Kollektiv von 2433 Männern, in dem wir 7 stetige Risikovariablen für die kardiovaskulären Erkrankungen untersuchten. Wir benutzten vor allem die Mahalanobis-Abstände und die zwei ersten und die zwei letzten Hauptkomponenten.

In dieser Arbeit prüfen wir das Problem: Was passiert mit den Ausreißern, wenn wir die Daten transformieren mit der Box-Cox Formel? Werden wir dieselben Ausreißer finden?

Es zeigt sich, daß wir von den transformierten Daten ganz andere Ausreißer bekommen können. Es tröstet uns jedoch, daß in jedem Fall die sehr großen Ausreißer gefunden werden.

1. The problem

In our earlier work (BARTKOWIAK et al., 1987) we have been considering some epidemiological data collected during the Wroclaw Coronary Heart Disease Primary Prevention Study subjected to the ERICA (European Risk and Incidence Coordinated Analysis) programme coordinated by the WHO Collaborating Centre in Heidelberg.

In particular, we considered seven Coronary Heart Disease (CHD) risk variables: 1. Body weight; 2. Systolic blood pressure I, accidental; 3. Diastolic blood pressure I, accidental; 4. Systolic blood pressure II, measured in standard conditions; 5. Diastolic blood pressure II, measured in standard conditions; 6. Cholesterol; 7. Glucose. These variables were observed in n = 2433 men aged 25–60 working in industrial plants of Wroclaw. Using various statistical methods (χ^2 plots calculated with ordinary and robust covariance matrices, diagonal elements of the HAT matrix considered as leverage points, scatter-diagrams of the first two and last two principal components) we located about 17 more or less serious outliers. The method using principal components was the most appealing.

The considered variables $X_1, \ldots, X_7$, especially the variables X_6 (cholesterol) and X_7 (glucose) were not normal. In particular, the variables X_6 and X_7 were very long-tailed. In Table 1 we present the means, standard, deviations, coefficients of asymmetry *as* and kurtosis *k* calculated from our data. The coefficients as and k were calculated using the formulae

$$as = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^3}{s^3}, \qquad (1)$$

$$k = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^4}{s^4} - 3,$$

Table 1. General statistical characteristics for the considered variables before and after transformation

Variable [unit]	mean $\bar{x}$	stand. dev. s	asym. *as*	kurtosis *k*	transformation
1. Body weight [kg]	77.6	11.1	0.36	0.4	untransformed
2. Syst. BP I	133.5	20.1	0.85	1.6	untransformed
[mm Hg]	4.88	0.15	0,30	0.47	transf. $\lambda = 0.0$
3. Diast. BP I [mm Hg]	85.3	12.2	0.57	1.1	untransformed
4. Syst. BP II	130.7	19.6	0.86	1.5	untransformed
[mm Hg]	4.86	0.15	0.32	0.42	transf. $\lambda = 0.0$
5. Diast. BP II [mm Hg]	83.8	12.0	0.62	1.1	untransformed
6. Cholesterol	230.3	44.6	1.36	11.0	untransformed
[mg %]	5.42	0.19	−0.01	1.26	transf. $\lambda = 0.0$
7. Glucose	99.0	25.9	7.4	94.9	untransformed
[mg %]	1.56	0.01	0.58	8.62	transf. $\lambda = -0.6$

with $\bar{x}$ and s being the appropriate mean and standard deviation.

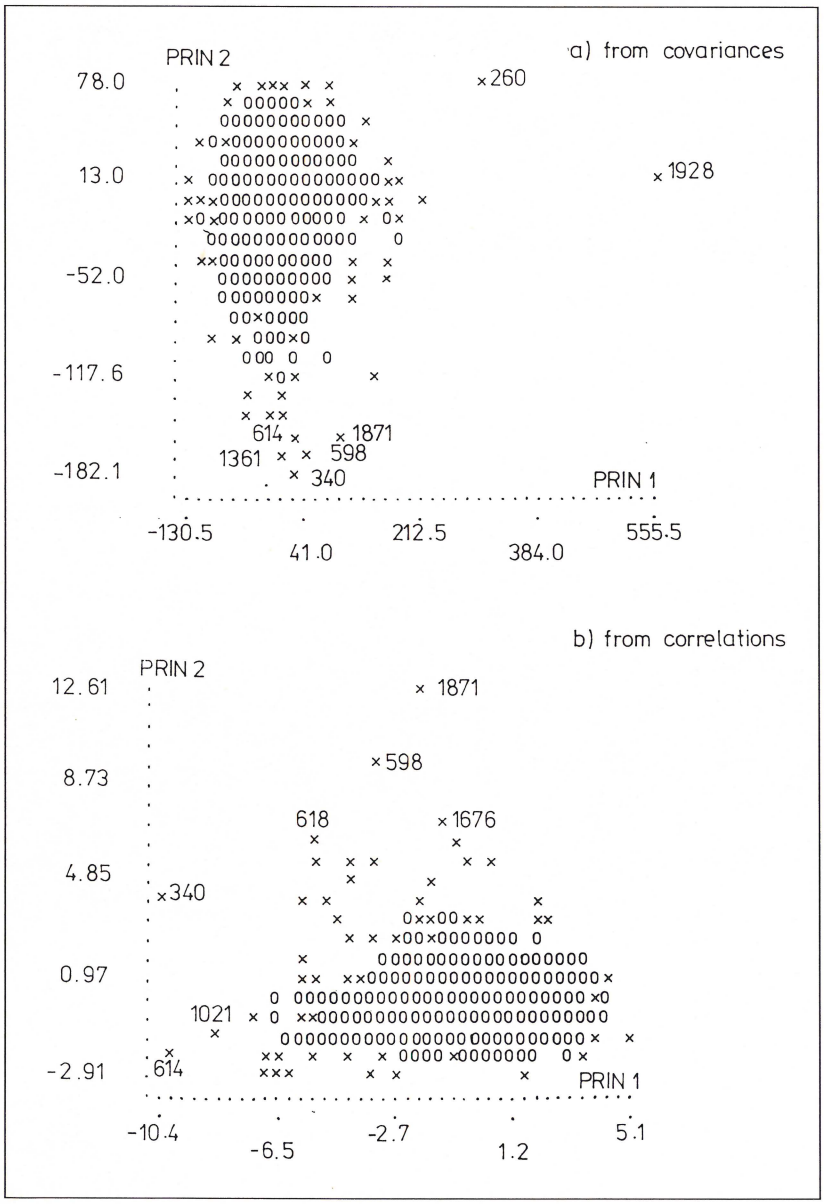
One can see that these coefficients are so defined that – for data subjected to the normal distribution – their expections are equal to 0.

Our problem is: Could the considered variables by use of some transformations be brought nearer to normality? If yes, what happens with the outliers? Could they still be identified using the first two and last two principal components?

2. Principal components from rescaled (linearly transformed) data

First we made a rescaling of the variables X_6 and X_7 dividing them by 10. This meant, that now these variables were expressed in mg%.

Fig. 1. Scatterdiagrams of the first two principal components evaluated using covariances and correlations calculated from rescaled data



For this rescaled set of data we recalculated the covariance matrix and the correlation matrix and next, on the basis of these matrices, the principal components. The scatterdiagram of the first two principal components (PRIN1, PRIN2) is given in Figure 1. Part a) of this figure shows the scatterdiagram of PRIN1 and PRIN2 obtained from the covariance matrix. Analogous scatterdiagram of PRIN1 and PRIN2 obtained from the correlation matrix is shown in part b) of Figure 1.

We see, that the scatterdiagrams shown in part a) and part b) look quite different. In part a) we see distinctly as outliers the points-individuals no. 1928 and 260. Gathering part b) it is hard to say, which points can be thought as outliers. The points no. 1871, 598, 340, 614, 618 and 1676 have the most extreme position. The two scatterdiagrams presented now look quite different as those presented in our former paper (BARTKOWIAK et al., 1987).

We do not show here the scatterdiagrams of PRIN6 and PRIN7, the last two principal components. They look much alike each to the other and also alike to those shown in our former paper. On the basis of these scatterdiagrams we can identify the points no. 369, 1141, 589 and 777.

The points mentioned above, except no. 340 and 614, were discovered previously, when considering unscaled data. On the other side, the points 340 and 614 were not seen, previously. It follows, that after rescaling the data (expressing the variables in other units) we can obtain much different scatterdiagrams of the first two and last two principal components. On the basis of these scatterdiagrams we identified some points-individuals which could be suspected to be outliers. These points are listed in Table 2 together with their normalized values.

We shall return to this table after finding analogous outstanding observations in scatterdiagrams of principal components obtained for transformed data.

3. The Box-Cox transformations and checking normality of the distributions

We considered the Box-Cox transformations defined as follows (BOX and COX, 1964):

$$y = \begin{cases} \dfrac{x^{\lambda} - 1}{\lambda} & \lambda \neq 0, \\ \ln(x) & \lambda = 0. \end{cases}$$

In the formula above »x« is the value before transformation, and »y« is the value after transformation.

Our goal was to reduce the kurtosis and asymmetry. For a given variable we tried various values of λ and retained that λ which gave the smallest (possibly nonnegative) values of the coefficients of asymmetry and kurtosis given by eq. (1).

After some trials we decided to retain the value $\lambda = 0.0$ for the variables X_2, X_4, X_6 and the value $\lambda = -0.6$ for the variable X_7. The statistical characteristics of the transformed

distributions are given also in Table 1, together with the appropriate values obtained from untransformed data. Looking at the Table 1 we see that the largest deviation from normality was exhibited by the variable X_7 (glucose). It has an enormous coefficient of kurtosis ($k = 94.9$!) and also a considerably large coefficient of asymmetry ($as = 7.4$). The variable X_6 (cholesterol) has also quite a large coefficient of kurtosis ($k = 11.0$) and a moderate coefficient of asymmetry ($as = 1.4$). The variables X_2 and X_4 (systolic blood pressure, accidental and in standard conditions) have rather a moderate k and as, none the less we succeeded in diminishing them more.

To visualize the effect of the transformations we use the technique of normal probability plots (BURY, 1975) called in the following shortly normal plots.

To draw a normal plot for given values $x_1, x_2, \ldots, x_n$ we first order these values to a nondecreasing sequence $x_{(1)} \leq x_{(2)} \leq \ldots \leq x_{(n)}$. Next, for each value $X_{(j)}$, we evaluate the quantile $q_j = F^{-1}(j/(n+1))$, F(.) being the cumulative probability distribution function of the Gauss-Laplace random variate. Drawing q_j against $x_{(j)}$ we obtain the normal plot. If the underlying distribution is normal then the points in the normal plot should be situated approximately along a straight line. Deviations from normality cause curvilinearity of the statistical dependence of the quantile q_j from the observed value $x_{(j)}$.

In Figure 2 we show normal probability plots for the variable X_7. Plots for other variables are much more regular; in particular the plots for the variables X_1–X_5 are nearly linear (we do not show them in this paper).

Looking at the Figure 2 part a) one has no doubts that the distribution is not normal. We see here also for large values of X_7 3 isolated points: no. 1361, 598 and 1871. These are clearly outliers with very big values in glucose. All they can be seen in Figure 1 part a). Two of them can be also seen in Figure 1 part b) and Figure 4 part b).

Looking at the Figure 2 part b) we state that after the transformation the curvilinearity is smaller, none the less it is still far from linearity. Now we see two isolated points (no. 1133 and 1173) of glucose. These points were not discovered so far.

4. Principal components from transformed data

In the following the partially transformed data (i.e. X_1, X_3, X_5 untransformed and X_2, X_4, X_6, X_7 transformed by the formula (2) with $\lambda = 0,0,0,-0.6$ appropriately) we shall call the transformed data.

Considering these transformed data we calculated the eigenvectors which were the basis for evaluation the principal components. In Table 3 we show the first two and last two eigenvectors obtained from:

a) covariances calculated from rescaled data;
b) correlations calculated from rescaled data;
c) covariances calculated from the partially transformed data;
d) correlations calculated from transformed data.

We see that the components of the vectors obtained from different matrices look quite different. Let us remind that the k-th principal component (PRINK), $k = 1, \ldots, p$ is evaluated from a properly rescaled data vector $\tilde{x} = (\tilde{x}_1, \ldots, \tilde{x}_p)$ using the formula

$$\text{PRINK} = \tilde{x}\, a_k, \tag{3}$$

where $a_k = (a_{i1}, \ldots, a_{ik})'$ is the k-th eigenvector and the rescaling of the data vector $x = (x_1, \ldots, x_p)$ means

a) for principal components calculated from covariances: subtraction of mean values: $\tilde{x} = x - \bar{x} = (x_1 - \bar{x}_1, \ldots, x_p - \bar{x}_p)$;
b) for principal components calculated from correlations: subtraction of mean values and dividing by standard deviations:

$$\tilde{x} = \frac{x - \bar{x}}{s} = \left(\frac{x_1 - \bar{x}_1}{s_1}, \ldots, \frac{x_p - \bar{x}_p}{s_p}\right)$$

Fig. 2. Normal plots for X_7 (glucose) before and after applying the Box-Cox transformations

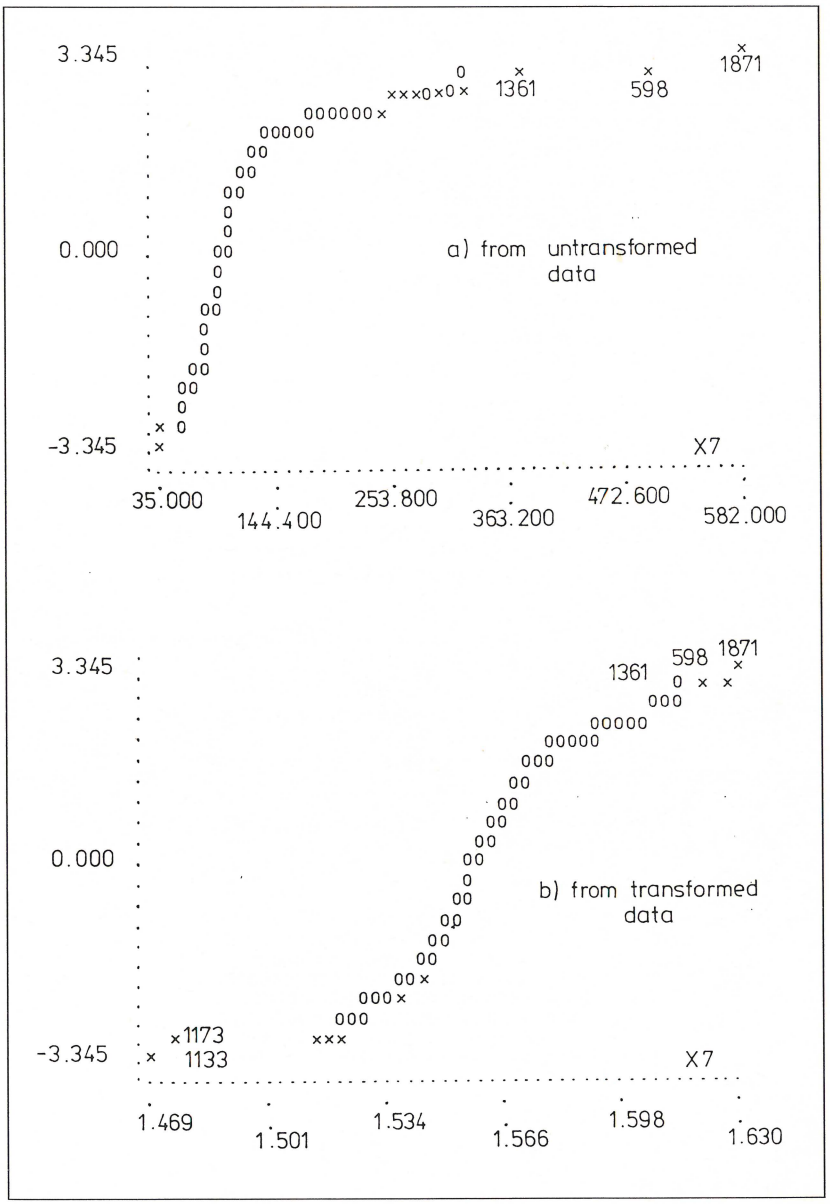


Table 2. Individuals found at outstanding positions in scatterdiagrams constructed from principal components (PC) obtained from rescaled data
A – identified by the first two PC (from covariances), B – identified by the first two PC (from correlations), C – identified by the last two PC (from covariances), D – identified by the last two PC (from correlations), F – identified in our former paper

(i)	z_{i1}	z_{i2}	z_{i3}	z_{i4}	z_{i5}	z_{i6}	z_{i7}	source				
143	not identified											
260	.8	−1.2	−1.3	−1.3	−1.2	6.8	−.4	A				
340	3.6	3.5	5.3	4.0	5.9	−.0	5.6	A	B			
369	.3	−1.8	−2.4	−1.6	.5	−.4	−.5			C	D	F
589	−1.9	−1.2	−.0	2.0	3.0	.6	−.9			C		F
598	−1.0	2.3	1.2	−.0	.5	.2	15.4	A	B		D	F
614	.0	5.8	5.3	5.1	4.7	.0	−.5	A	B			
618	1.1	2.6	3.6	1.0	1.3	2.7	7.9		B			F
713	not identified											
757	.6	2.3	3.7	1.5	.5	−.1	.0			C		
777	3.1	−.2	−.4	2.0	−.3	.7	2.6			C	D	F
848	not identified											
1021	.0	4.8	3.7	5.1	3.9	−.0	.3		B			
1133	not identified											
1141	.5	1.8	−1.3	1.5	1.3	.3	.2			C	D	F
1173	not identified											
1361	−.9	2.3	2.0	2.5	2.2	−.4	10.7	A				F
1676	.4	.4	−.4	.2	−.3	3.5	7.4		B			F
1860	not identified											
1861	not identified											
1871	−.5	.1	.4	−.8	.1	1.3	18.7	A	B			F
1915	not identified											
1928	−.6	1.8	1.2	1.5	1.3	12.4	.5	A				F

Looking at the components of the eigenvectors, especially at those calculated from the correlation matrices, we can judge which variables are influential for the calculated principal components: namely these are influential, for which the appropriate components in the eigenvectors are big.

Looking at the Table 1 we can infer that:

A) The first two principal components calculated from covariances obtained from rescaled data are influenced mostly by X_6 (PRIN1) and X_2, X_3, X_4, X_5, X_7 (PRIN2).

B) The first two principal components calculated from correlations obtained from rescaled data are influenced mostly by X_2, X_3, X_4, X_5 (PRIN1) and X_1, X_6, X_7 (PRIN2).

C) The first two principal components calculated from covariances obtained from transformed data are influenced mostly by X_2, X_4 (PRIN1) and X_1 (PRIN2).

D) The first two principal components calculated from correlations obtained from transformed data are influenced mostly by X_2, X_3, X_4, X_5 (PRIN1) and X_1, X_6, X_7 (PRIN2).

It follows that scatterdiagrams of PRIN1, PRIN2 calculated from various kinds of matrices will reflect different properties of the data and are likely to show different outliers.

The same inference can be drawn after inspecting the components of the last two eigenvectors.

In Figure 3 we show scatterdiagrams of the first two (PRIN1, PRIN2) and last two (PRIN6, PRIN7) principal components evaluated using covariances from the transformed data.

In Figure 4 we show scatterdiagrams of the analogous principal components evaluated using correlations from the transformed data.

We see that now, for the transformed data, the scatterdiagrams look quite different as those obtained formerly for untransformed data.

On the basis of these scatterdiagrams we identify some points which can be suspected to be outliers. These points are listed in Table 4 together with their normalized values.

5. Comments on the identified outliers

Looking at the standardized values of the individuals found at outstanding positions in the scatterdiagrams we can state, that each of these individuals has some untypical features. Some individuals have simply unusually large values in some variables, other individuals exhibit unproportional values between some of the blood pressure measurements: either the accidental blood pressure readings differ much from analogous readings recorded in standard conditions, either one of these readings differs much from the others.

Scatterdiagrams constructed from transformed data are generally more symmetric. We found here some outliers not detected formerly when considering the first two and last two principal components from untransformed data. In particular

Table 3. First two and last two eigenvectors calculated from the covariance and correlation matrices evaluated for rescaled and transformed data

vector component	a_1	a_2	a_6	a_7
A) covariances calculated from rescaled data				
1	0.0183	−0.0889	0.0137	0.0021
2	0.0576	−0.5877	0.6032	0.3293
3	0.0301	−0.3138	0.3568	−0.5996
4	0.0565	−0.5715	−0.6348	−0.3511
5	0.0309	−0.3073	−0.3247	0.6394
6	0.9935	0.1094	0.0011	−0.0006
7	0.0649	−0.3394	−0.0149	−0.0043
B) correlations calculated from rescaled data				
1	−0.1616	0.5262	0.0065	−0.0031
2	−0.4901	−0.0847	0.4146	−0.5627
3	−0.4865	−0.0994	0.5756	0.4045
4	−0.4925	−0.0989	−0.4162	0.5810
5	−0.4877	−0.1016	−0.5684	−0.4267
6	−0.0509	0.5107	0.0047	0.0011
7	−0.1183	0.6520	−0.0190	0.0118
C) covariances calculated from transformed data				
1	−0.2363	0.9717	−0.0000	−0.0002
2	−0.0065	−0.0013	−0.6963	−0.0094
3	−0.6944	−0.1711	0.0036	0.0000
4	−0.0066	−0.0013	0.7177	−0.0003
5	−0.6796	−0.1630	−0.0039	−0.0000
6	−0.0007	0.0006	−0.0012	−0.0045
7	−0.0001	0.0002	−0.0063	0.9999
D) correlations calculated from transformed data				
1	−0.1652	0.5393	−0.0040	−0.0018
2	−0.4883	−0.1010	−0.4197	−0.5575
3	−0.4852	−0.1093	−0.5714	0.4128
4	−0.4913	−0.1005	0.4264	0.5752
5	−0.4865	−0.1050	0.5616	−0.4335
6	−0.0535	0.4892	−0.0054	−0.0007
7	−0.1340	0.6531	0.0028	0.0037

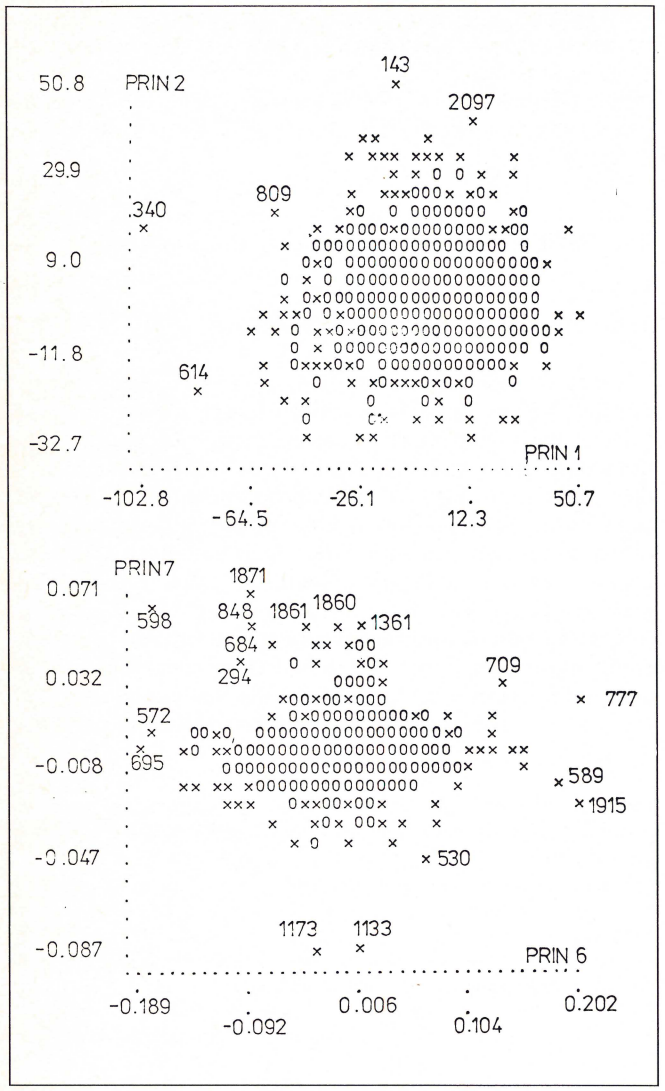


Fig. 3. Scatterdiagrams of PRIN1, PRIN2, the first two and PRIN6, PRIN7, the last two principal components evaluated using covariances from transformed data

we have found here individuals (no. 1133 and 1173) which have very small values of glucose ($t = -8.3$ and $t = -7.7$). None the less, the most severe outliers were found in untransformed and transformed data as well.

6. Detection of outliers with Mahalanobis distances evaluated for the transformed data

Similarly, as in our former paper, we evaluated for the transformed data the Mahalanobis distances of each individual from the centroid of the cluster of points-individuals, ordered these distances and constructed the χ^2-plot. It is not so much curvilinear as formerly. The five most outstanding points are: no. 589, no. 598, no. 1173 (N), no. 777, no. 1133 (N) and, except no. 598, are different from those find at the top of the χ^2-plot presented in our former paper. The individuals no. 589 and no. 777 were put previously at the 7th and 12th places. The individuals no. 1173 and no. 1133 are as outliers new: they were detected only when using transformed data.

Repeating the calculations with robust covariance matrices (trimming a fraction of individuals with the largest Mahalanobis distances, computing a weighted covariance matrix using Huber's or Hampel's weights) gave nothing essentially new; only the most extreme points were separated a little more from the remaining ones.

7. Final conclusions

The first two and last two principal components can be very useful for detection and identifying outliers.

It can happen that these principal components allow to detect outliers only in some variables. This can be foreseen after gathering at the components of the eigenvectors which serve as the basis for the evaluation of the principal components.

Fig. 4. Scatterdiagrams of PRIN1, PRIN2, the first two and PRIN6, PRIN7, the last two principal components evaluated using correlations from transformed data

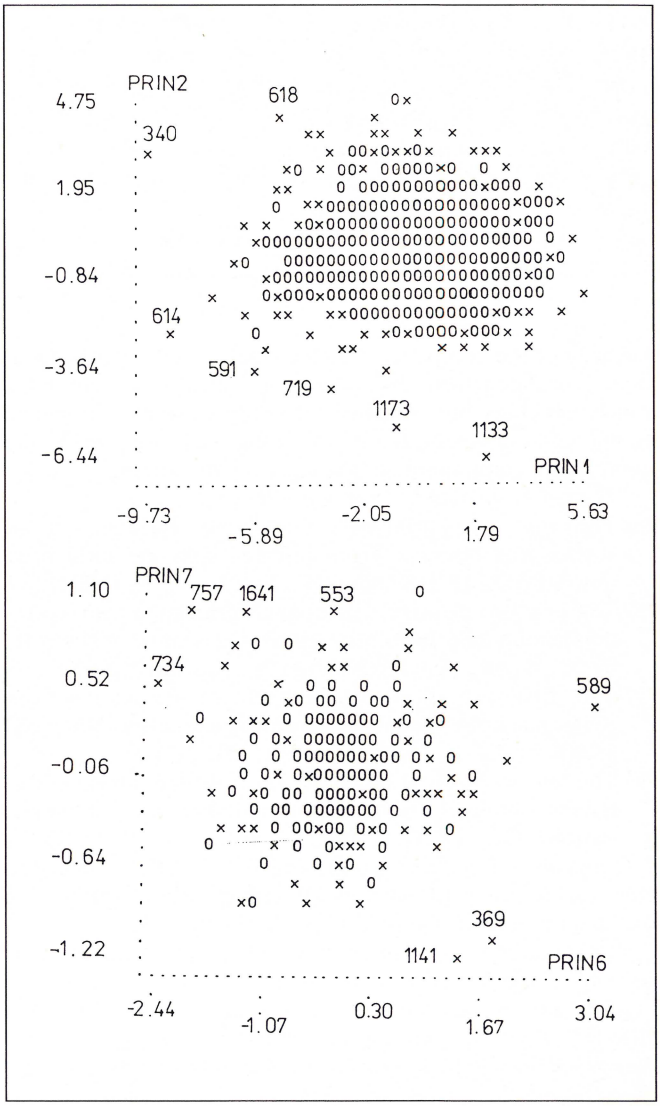


Table 4. Individuals found at outstanding positions in scatterdiagrams constructed from principal components (PC) obtained from transformed data
A – identified by the first two PC (from covariances), B – identified by the first two PC (from correlations), C – identified by the last two PC (from covariances), D – identified by the last two PC (from correlations), F – identified in our former paper

(i)	z_{i1}	z_{i2}	z_{i3}	z_{i4}	z_{i5}	z_{i6}	z_{i7}	Source				
143	4.7	1.3	–.0	1.0	.0	.1	1.3	A				
260	not identified											
340	3.6	3.0	5.3	3.3	5.9	.1	4.2	A	B			
369	.3	–2.0	–2.5	–1.8	–.5	–.3	–.7				D	F
589	–2.0	–1.2	–.0	1.9	3.0	.7	–1.6			C	D	F
598	–1.0	2.1	1.2	.0	–.5	.3	6.2			C		F
614	.0	4.4	5.3	4.0	4.7	.1	–.8	A	B			
618	1.1	2.3	3.7	1.0	1.3	2.3	4.9		B			F
713	–.5	2.1	2.0	2.1	1.3	–2.3	–3.0		B			
757	.6	2.1	3.7	1.5	–.5	–.0	.2				D	
777	3.1	–.1	–.4	1.9	–.3	.8	2.8			C		F
848	.0	2.1	2.7	1.5	3.0	–1.5	5.1				D	F
1021	not identified											
1133	–.9	–.7	–.4	–.5	–.3	–1.6	–8.3		B	C	D	
1141	.5	1.7	–1.3	1.5	1.3	.4	.5				D	F
1173	.9	1.5	.4	1.2	.5	–.8	–7.7		B	C	D	
1361	–.9	2.1	2.0	2.3	2.2	–.3	5.6					F
1676	not identified											
1860	.7	–.4	1.3	–.5	–1.2	–.1	5.0				D	F
1861	.8	.4	–.8	.0	–.7	–.2	5.1				D	F
1871	–.5	.1	.4	–.8	.1	1.3	6.6			C		F
1915	–.9	–1.4	–1.3	.5	–1.2	–1.4	–2.6			C		
1928	not identified											

Transformation of the data – performed with the aim to bring the distributions nearer to normality – makes generally the scatterdiagrams more symmetric. Very big outliers (very big values in a long-tailed distribution) can after the appropriate transformation be absorbed and swamped with other values.

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Date of receipt: 14. 03. 88
The authors' addresses: Dr. Anna Bartkowiak, Inst. of Computer Science, University of Wroclaw, Przesmyckiego 20, Wroclaw 51-151, Poland. Prof. Dr. S. Lukasik, Dr. K. Chwistecki, Dr. M. Mrukowicz, Dept. of Cardiology, Medical Academy, Pasteura 4, Wroclaw 50-367, Poland. Wolfgang Morgenstern, Institute of Clinical Social Medicine, University of Heidelberg, Bergheimer Str. 58, Heidelberg 6900, Federal Republic of Germany

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Analysis of offsprings of a diallel experiment in a BIB design – A mixed model

Bronisław Ceranka and Stanisław Mejza

Summary

In this paper the analysis of genotypes from a diallel crossing system including sets of offsprings and reciprocals is given. The analysis is presented for data obtainable from a BIB design experiment in which the block effects are considered as random. The statistical analysis includes analysis of variance and the estimation (intra-block, inter-block and combined) of general and specific combining abilities and of reciprocal effects. Also tests of certain hypotheses concerning some genetical parameters are given.

Zusammenfassung

Die Arbeit enthält die Genotypenanalyse mit Hilfe dialleler Kreuzungssysteme einschließlich reziproker Kreuzungen. Die Auswertung erfolgt für Daten aus balancierten unvollständigen Blockanlagen, wobei die Blockeffekte als zufällig angesehen werden. Die statistische Auswertung umfaßt die Varianzanalyse und die Schätzung der allgemeinen und spezifischen Kombinationseignung und der reziproken Effekte. Ferner werden Tests von Hypothesen bezüglich einiger genetischer Parameter angegeben.

1. Introduction

The diallel crossing system is often of interest for breeders dealing with estimation and testing of general and specific combining abilities and reciprocal effects. In this paper we consider one type of diallel crossing system, type III according to the classification by GRIFFING (1956). This type of diallel crossing includes F_1s and the reciprocal of F_1s, but not the parents.

GRIFFING (1956) gave the analysis of the general and specific combining abilities some genetical characteristics for data obtainable in a randomized block design only. In this paper the generalization of the analysis of GRIFFING's (1956) type III crossing system concerns the sampling nature of the experimental material. In particular, a method of analysing of the considered genetical characteristics for experiments laid out in a balanced incomplete block (BIB) design is given. It is assumed that genotype effects determined by the diallel crossing system are fixed. But for block effects it is assumed that they are random. According to the GRIFFING's (1956) notation concerning sets of assumptions which can be considered with regard to the genotype and block effects, the set (3) is taken into account. The situation in which both the genotype and the block effects were fixed (i.e. the case of GRIFFING's set (1) of assupmtions) was considered by CERANKA and KIEŁCZEWSKA (1985). Results of that paper will be helpful here.

It would be also interesting to see other papers concerning some problems connected with analysis of diallel tables. In particular CERANKA and KIEŁCZEWSKA (1986 b, a) give the analysis of genotypes for types I and II of GRIFFING's classification, for experiments laid out in block designs. Analysis in those papers is based on a classical fixed model, i.e. the model in which the genotype and the block effects are fixed.

The similar approach to the analysis of diallel table as in this paper (i.e. a mixed model) is used by CERANKA and MEJZA (1987, 1988). In particular in those papers the types II and I are considered, respectively.

2. The analysis of a mixed model

Let y be an $n \times 1$ vector of observations from an experiment in which v treatments are applied to n plots arranged in b blocks of size k each. The linear model for data obtained in such a block design may be written in the form

$$(2.1) \quad y = \mu 1 + \Delta'\tau + D'\beta + \eta,$$

where 1 is the $n \times 1$ unit vector, Δ' is an $n \times v$ design matrix for treatments, D' is an $n \times b$ design matrix for blocks, so that $N = \Delta D'$ is the $v \times b$ incidence matrix of the design, μ is a general parameter, τ is the $v \times 1$ vector of treatment parameters, β is the $b \times 1$ vector of block parameters and η is the $n \times 1$ vector of residuals. It is assumed that vectors β and η are random and that they are normally distributed with $E(\beta) = 0$, $E(\eta) = 0$, $E(\beta\beta') = \sigma_b^2 I$, $E(\eta\eta') = \sigma^2 I$ and $E(\beta\eta') = 0$, where I is the identity matrix of conformable order. Hence, $Cov(y) = \sigma^2 I + \sigma_b^2 D'D$.

In the analysis of model (2.1) the variance components σ^2 and σ_b^2 play an important role. In particular, which of the methods of estimation is to be used depends on whether σ^2 and σ_b^2 are known or not. Practically the variance components σ^2 and σ_b^2 are not known. Such a situation will be considered here. In this case the so-called intra- and inter-block analyses are very helpful in the analysis of results based on model (2.1).

In this paper we will consider BIB designs only, for which estimation and testing of hypotheses will be restricted to

contrasts of treatment parameters, i.e., to linear functions $c'\tau$, where $c'1 = 0$. This is fair enough, because it can be proved that if a linear function of treatment parameters is estimable then it must be a contrast.

It can be shown (see: MEJZA, 1985) that the so-called intra-block estimator of contrast of treatment parameters in a BIB design with r treatment replications is of the form

$$(2.2)\quad \hat{c'\tau} = (k/(\lambda v))Q,$$

where $\lambda = r(k-1)/(v-1)$ and $Q = (\Delta - (1/k)ND)y$, and that under model (2.1) it is an unbiased estimator of $c'\tau$. In the formula (2.2) the vector Q can also be written $Q = T - (1/k)NB$, where $T = \Delta y$ is the $v \times 1$ vector of treatment totals, and $B = Dy$ is the $b \times 1$ vector of block totals. The variance of $\hat{c'\tau}$ is $\mathrm{Var}(\hat{c'\tau}) = (k/(\lambda v))c'c\sigma^2$, and σ^2 can be estimated by $s_E^2 = E/(n-b-v+1)$, where $E = y'y - (1/k)B'B - (k/(\lambda v))Q'Q$ is the sum of squares due to error in the intra-block analysis.

Since the analysed combining abilities and reciprocal effects are expressible in terms of contrasts of treatment parameters, it is sufficient to consider the testing of hypotheses concerning contrasts. Suppose we consider h independent contrasts of treatment parameters, $c_1'\tau, \ldots, c_h'\tau$, where $c_i'1 = 0$ for $i = 1, \ldots, h$. If we are interested in testing the hypothesis H_o: $C'\tau = 0$, where $C = [c_1, \ldots, c_h]$, with rank $C = h$, then the appropriate F-statistic is

$$(2.3)\quad F = \frac{kQ'\,C(C'C)^{-1}\,C'Q}{\lambda v h s_E^2}.$$

If we are interested in testing a hypothesis concerning an individual contrast $c'\tau$, i.e. a hypothesis H_o: $c'\tau = 0$, then the appropriate F-statistic is

$$(2.4)\quad F = \frac{\lambda v(\hat{c'\tau})^2}{k s_E^2 c'c}.$$

Now, we will consider the estimation of contrasts of treatment parameters in the so-called inter-block analysis. It can be shown that the estimator of that contrast in a BIB design has the form

$$(2.5)\quad \tilde{c'\tau} = (1/(r-\lambda))c'NB,$$

and that it is an unbiased estimator of $c'\tau$ under model (2.1). The variance of $\tilde{c'\tau}$ is $\mathrm{Var}(\tilde{c'\tau}) = (1/(r-\lambda))c'c\sigma_o^2$, and an unbiased estimator of the inter-block variance $\sigma_o^2 = \sigma^2 + k\sigma_b^2$ is $\hat{\sigma}_o^2 = s_{E_o}^2 = E_o/(b-v)$, where $E_o = (1/k)B'B + (\lambda/(r(r-\lambda)))(B'1)^2 - (1/(k(r-\lambda)))B'N'NB$ is the sum of squares due to error in the inter-block analysis. In this case, for testing of the hypothesis H_o: $C'\tau = 0$, rank $C = h$, the F-statistic

$$(2.6)\quad F_o = \frac{B'N'C(C'C)^{-1}\,C'NB}{h(r-\lambda)s_{E_o}^2},$$

can be used.

If we are interested in testing a hypothesis described by an individual contrast $c'\tau$, i.e. a H_o: $c'\tau = 0$, then the appropriate F-statistic is

$$(2.7)\quad F_o = \frac{(r-\lambda)\,(\tilde{c'\tau})^2}{c'c\; s_{E_o}^2}.$$

It can be shown that the intra- and the inter-block estimators are under model (2.1) distributed independently. This property can be utilized for combining the unbiased estimators. In the literature one can find several methods of combining estimators. In this paper the method given by MEJZA (1978) will be used.

Let us consider a set of h contrasts of treatment parameters $c_i'\tau$, $i = 1, \ldots, h$, and let $\hat{c_i'\tau}$ and $\tilde{c_i'\tau}$ be the intra- and the inter-block estimator of $c_i'\tau$, respectively. According to our assumptions, we have $\hat{c_i'\tau} \sim N(c_i'\tau, d_i\sigma^2)$ and $\tilde{c_i'\tau} \sim N(c_i'\tau, e_i\sigma_o^2)$, $i = 1, \ldots, h$, where $d_i = (k/(\lambda v))c_i'c_i$ and $e_i = (1/(r-\lambda))c_i'c_i$. Then the combined estimator

$$(2.8)\quad \hat{c_i'\tau} = \tilde{c_i'\tau} + (\tilde{c_i'\tau} - \hat{c_i'\tau})\,\frac{d_i(h-2)s_E^2}{\sum_{i=1}^{h}(\tilde{c_i'\tau} - \hat{c_i'\tau})^2}$$

is uniformly better than $\tilde{c_i'\tau}$, i.e. $\mathrm{Var}(\hat{c_i'\tau}) \le \mathrm{Var}(\tilde{c_i'\tau})$, provided $h > 2$ and $n-b-v+1 > 0$, and hence the combined estimators are recommended in the paper.

Analogously, a combined test of the hypothesis H_o: $c_i'\tau = 0$ will be used. The combined test is based on the F-tests obtained in the intra- and the inter-block analyses. LITTEL and FOLKS (1973) proved that a test obtained by Fisher's method of combining tests is asymptotically optimal, with respect to Bahadur's relative efficiency, among essentially all methods of combining independent tests, and hence this test will be recommended here. According to Fisher's method, the statistic

$$(2.9)\quad z = -2 \log PP_o,$$

where P is the significance level of F given in (2.4) and P_o is that of F_o given in (2.7), is distributed as a χ^2 variable with 4 degrees of freedom.

3. The analysis of genetical parameters

3.1 Model

For the considered type of diallel crossing system, the number of genotypes (treatments) is $v = p(p-1)$, where p is the number of parental lines. Let us denote the vector of genotype effects by $\gamma = [\gamma_{12}, \ldots, \gamma_{p-1,p}]'$, where $\gamma = \mu 1 + \tau$, with μ and τ defined as in (2.1). The elements of vector γ can most conveniently be set out in a table of the form

$$\begin{array}{cccccc}
 & \gamma_{12} & \gamma_{13} & \cdots & \gamma_{1,p-1} & \gamma_{1p} \\
\gamma_{21} & & \gamma_{23} & \cdots & \gamma_{2,p-1} & \gamma_{2p} \\
\gamma_{31} & \gamma_{32} & & \cdots & \gamma_{3,p-1} & \gamma_{3p} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\gamma_{p1} & \gamma_{p2} & \gamma_{p3} & \cdots & \gamma_{p-1,p} &
\end{array},$$

where γ_{ij}, $i < j = 1, \ldots, p$, represents the effect of the genotype resulting from crossing the ith and the jth inbreds and γ_{ji} represents its reciprocal.

The model for the effects γ_{ij} is assumed to be

$$\gamma_{ij} = \mu + g_i + g_j + s_{ij} + w_{ij}, \quad i, j = 1, \ldots, p,\ i \neq j$$

where μ is the general parameter, g_i (g_j) is the general combining ability (g.c.a.) for the ith (jth) parent, s_{ij} is the specific combining ability (s.c.a.) for the cross between the parents ith and the jth, such that $s_{ij} = s_{ji}$, and w_{ij} is the reciprocal effect involving the cross between the parents jth and ith, such that $w_{ij} = -w_{ji}$. It will be assumed that $\sum_i g_i = 0$ and that $\sum_{i \neq j} s_{ij} = 0$ for each j.

3.2. Estimation

As mentioned before, the estimation of genetical parameters will base on combining estimators. According to the method of combining estimators given by MEJZA (1978), we can write the combined estimators of considered genetical parameters as follows.

The combined estimator of g_i is

$$\tilde{g}_i = \hat{g}_i + (\tilde{g}_i - \hat{g}_i)\frac{k(p-1)(p-3)s_E^2}{2\lambda\, vp(p-2)\sum_{i=1}^{p}(\tilde{g}_i-\hat{g}_i)^2},$$

where $\hat{g}_i$ is the intra-block estimator of g_i, of the form

$$\hat{g}_i = \frac{1}{2p(p-2)}[p(\hat{\gamma}_{i.} + \hat{\gamma}_{.i}) - 2\hat{\gamma}_{..}],$$

with

$$\hat{\gamma}_{i.} = \sum_j \hat{\gamma}_{ij}, \quad \hat{\gamma}_{ji} = \hat{\gamma}_{ij},$$

and

$$\hat{\gamma}_{..} = \sum_i \sum_j \hat{\gamma}_{ij},$$

obtainable from $\hat{\gamma} = (k/(\lambda\ v))Q + (G/n)1$, where $G = T'1 = B'1$, and where $\tilde{g}_i$ is the inter-block estimator of g_i, which can be obtained when replacing $\hat{\gamma}$ by $\tilde{\gamma} = (1/(r-\lambda))\ (NB - (\lambda/r)G1)$ in the above formulae.

The combined estimator of s_{ij} is

$$\tilde{s}_{ij} = \hat{s}_{ij} + (\tilde{s}_{ij} - \hat{s}_{ij})\frac{k(p+1)(p-3)(p-4)s_E^2}{4\lambda v(p-1)\sum_{i=1}^{p}\sum_{j=i+1}^{p}(\tilde{s}_{ij}-\hat{s}_{ij})^2},$$

where for any pair i, j $(= 1, \ldots, p, i \neq j)$ $\hat{s}_{ij}$ is the intra-block estimator of s_{ij} of the form

$$\hat{s}_{ij} = \frac{1}{2}(\hat{\gamma}_{ij} + \hat{\gamma}_{ji}) - \frac{1}{2(p-2)}(\hat{\gamma}_{i.} + \hat{\gamma}_{.i} + \hat{\gamma}_{j.} + \hat{\gamma}_{.j}) + \frac{1}{(p-1)(p-2)}\hat{\gamma}_{..},$$

and $\tilde{s}_{ij}$ is the inter-block estimator of s_{ij}, which can be obtained again by replacing $\hat{\gamma}$ by $\tilde{\gamma}$.

The combined estimator of w_{ij} is

$$\tilde{w}_{ij} = \hat{w}_{ij} + (\tilde{w}_{ij} - \hat{w}_{ij})\frac{k(p+1)(p-4)s_E^2}{4\lambda v\sum_{\substack{i=1\\ i\neq j}}^{p}\sum_{j=1}^{p}(\tilde{w}_{ij}-\hat{w}_{ij})^2},$$

where for any pair i, j $(= 1, \ldots, p, i \neq j)$ $\hat{w}_{ij}$ is the intra-block estimator of w_{ij} of the form

$$\hat{w}_{ij} = \frac{1}{2}(\hat{\gamma}_{ij} - \hat{\gamma}_{ji})$$

and $\tilde{w}_{ij}$ is the inter-block estimator of w_{ij}, which can be obtained using $\tilde{\gamma}$ instead of $\hat{\gamma}$.

3.3 Testing hypotheses

In the analysis of combining abilities the interesting hypotheses concerning the g.c.a., s.c.a. and reciprocal effects can be formulated as follows:

1. H_o: $g_i = 0$; for all i,
2. H_o: $s_{ij} = 0$; for all $i \neq j$,
3. H_o: $w_{ij} = 0$; for all $i \neq j$,
4. H_o: $g_i = 0$; for fixed i,
5. H_o: $g_i - g_j = 0$; for fixed $i \neq j$,
6. H_o: $s_{ij} = 0$; for fixed $i \neq j$,
7. H_o: $s_{ij} - s_{ik} = 0$; $i \neq j, k$; $j \neq k$,
8. H_o: $s_{ij} - s_{kl} = 0$; $i \neq j, k, l$; $j \neq k, l$; $k \neq l$,
9. H_o: $w_{ij} = 0$; for fixed $i \neq j$,
10. H_o: $w_{ij} - w_{kl} = 0$; $i \neq j, k \neq l$,

where i, j, k, l, $= 1, \ldots, p$.

In the present paper, the combined test (2.9) will be used. With respect to the above, we need the significance levels of the appropriate F-tests used to test the same hypothesis. Now we will describe the two F-tests for each of the hypotheses 1–10.

For testing hypotheses 1–3 we use the F-statistics given in (2.3) and (2.6) which can now be expressed in explicit forms.

For testing the hypothesis 1, the F-statistics have the forms, and corresponding distributions,

$$F = \frac{2\lambda v(p-2)\ \hat{g}'\hat{g}}{k(p-1)s_E^2} \underset{\sim}{H_o} F(p-1,\ n-b-v+1)$$

and

$$F_o = \frac{2(r-\lambda)(p-2)\ \tilde{g}'\tilde{g}}{(p-1)s_{E_o}^2} \underset{\sim}{H_o} F(p-1,\ b-v),$$

in the intra- and the inter-block analysis, respectively, where $\hat{g} = [\hat{g}_1, \ldots, \hat{g}_p]'$ and $\tilde{g} = [\tilde{g}_1, \ldots, \tilde{g}_p]'$.

For testing the hypothesis 2, the F-statistics have the forms

$$F = \frac{2\lambda v\hat{s}'\hat{s}}{kp(p-3)s_E^2} \underset{\sim}{H_o} F(p(p-3)/2,\ n-b-v+1)$$

and

$$F_o = \frac{2(r-\lambda)\tilde{s}'\tilde{s}}{p(p-3)s_{E_o}^2} \underset{\sim}{H_o} F(p(p-3)/2,\ b-v),$$

in the intra- and inter-block analysis, respectively, where $\hat{s} = [\hat{s}_{12}, \ldots, \hat{s}_{p-1,p}]'$ and $\tilde{s} = [\tilde{s}_{12}, \ldots, \tilde{s}_{p-1,p}]'$.

For testing the hypothesis 3, the F-statistics have the forms

$$F = \frac{2\lambda v\hat{w}'\hat{w}}{kp(p-1)s_E^2} \underset{\sim}{H_o} F(p(p-1)/2,\ n-b-v+1)$$

and

$$F_o = \frac{2(r-\lambda)\tilde{w}'\tilde{w}}{p(p-1)s_{E_o}^2} \underset{\sim}{H_o} F(p(p-1)/2,\ b-v),$$

in the intra- and the inter-block analysis, respectively, where $\hat{w} = [\hat{w}_{12}, \ldots, \hat{w}_{p-1,p}]'$ and $\tilde{w} = [\tilde{w}_{12}, \ldots, \tilde{w}_{p-1,p}]'$.

For testing the hypotheses 4–10, the appropriate F-statistics given by (2.4) and (2.7) have

– for hypothesis 4 the forms

$$F = \frac{2\lambda vp(p-2)\hat{g}_i^2}{k(p-1)s_E^2}$$

and

$$F_o = \frac{2(r-\lambda)\ p(p-2)\tilde{g}_i^2}{(p-1)s_{E_o}^2},$$

– for hypothesis 5 the forms

$$F = \frac{\lambda v(p-2)(\hat{g}_i - \hat{g}_j)^2}{ks_E^2}$$

and

$$F_o = \frac{(r-\lambda)(p-2)(\tilde{g}_i - \tilde{g}_j)^2}{s_{E_o}^2},$$

– for hypothesis 6 the forms

$$F = \frac{2\lambda v(p-1)\hat{s}_{ij}^2}{k(p-3)s_E^2}$$

and

$$F_o = \frac{2(r-\lambda)(p-1)\tilde{s}_{ij}^2}{(p-3)s_{E_o}^2},$$

– for hypothesis 7 the forms

$$F = \frac{\lambda v(p-2)(\hat{s}_{ij} - \hat{s}_{ik})^2}{k(p-3)s_E^2}$$

and

$$F_o = \frac{(r-\lambda)(p-2)(\tilde{s}_{ij} - \tilde{s}_{ik})^2}{(p-3)s_{E_o}^2},$$

– for hypothesis 8 the forms

$$F = \frac{\lambda v(p-2)(\hat{s}_{ij} - \hat{s}_{kl})^2}{k(p-4)s_E^2}$$

and

$$F_o = \frac{(r-\lambda)(p-2)(\tilde{s}_{ij} - \tilde{s}_{kl})^2}{(p-4)s_{E_o}^2},$$

– for hypothesis 9 the forms

$$F = \frac{2\lambda v \hat{w}_{ij}^2}{ks_E^2}$$

and

$$F_o = \frac{2(r-\lambda)\tilde{w}_{ij}^2}{s_{Eo}^2},$$

– for hypothesis 10 the forms

$$F = \frac{\lambda v(\hat{w}_{ij} - \hat{w}_{kl})^2}{ks_E^2}$$

and

$$F_o = \frac{(r-\lambda)(\tilde{w}_{ij} - \tilde{w}_{kl})^2}{s_{E_o}^2}.$$

If the hypotheses 4–10 are true, then the F-statistics and F_o-statistics have the F-distributions with 1 and $n-b-v+1$ or 1 and $b-v$ degrees of freedom, respectively.

4. An example

For illustrating the theory given in this paper, let us consider, as an example, an experiment carried out in a balanced incomplete block design with $v = 12$ genotypes, resulting from the diallel crossing among $p = 4$ inbred lines of sunflower. In this experiment the diameter of capitulum was observed. The genotypes were allocated in $b = 33$ blocks of size $k = 4$. Each genotype was replicated $r = 11$ times in the experiment.

The first step in the analysis is to calculate the mean squares of errors in the intra- and the inter-block analyses, respectively. We obtain that $s_E^2 = 0.690$ and $s_{E_o}^2 = 0.448$.

The next step is the estimation of effects of genotypes in the intra- and the inter-block analyses, i.e. the calculation of the vectors $\hat{\gamma}$ and $\tilde{\gamma}$, respectively, the elements of which are arranged in the following tables:

– in the intra-block analysis the estimated genotype effects are

i \ j	1	2	3	4
1	–	15.58	13.60	17.11
2	10.51	–	16.11	15.81
3	17.52	18.82	–	15.05
4	12.63	13.27	13.81	–

– in the inter-block analysis the estimated genotype effects are

i \ j	1	2	3	4
1	–	15.85	13.00	16.00
2	12.53	–	15.77	15.52
3	17.21	18.62	–	14.73
4	12.57	13.03	14.97	–

Now, using the formulae given in section 3.2 we can estimate the g.c.a., s.c.a. and reciprocals effects. The estimates of g.c.a. effects are as follows:

– in the intra-block analysis they are
$\hat{g}_i = -0.74,\ \hat{g}_2 = 0.05,\ \hat{g}_3 = 1.25,\ \hat{g}_4 = -0.56,$

– in the inter-block analysis they are
$\tilde{g}_1 = -0.69,\ \tilde{g}_2 = 0.36,\ \tilde{g}_3 = 1.10,\ \tilde{g}_4 = -0.77,$

– in the combined analysis they are
$\bar{g}_1 = -0.74,\ \bar{g}_2 = 0.08,\ \bar{g}_3 = 1.24,\ \bar{g}_4 = -0.58.$

The estimates of the s.c.a. effects are arranged in tables:

– in the intra-block analysis the estimates are

i \ j	1	2	3	4
1	–	−1.25	0.07	1.18
2	−1.25	–	1.18	0.07
3	0.07	1.18	–	−1.25
4	1.18	0.07	−1.25	–

– in the inter-block analysis the estimates are

i \ j	1	2	3	4
1	–	−0.46	−0.29	0.76
2	−0.46	–	0.76	−0.29
3	−0.29	0.76	–	−0.46
4	0.76	−0.29	−0.46	–

– in the combined analysis the estimates are equal to those obtained in the intra-block analysis.

The estimates of the reciprocal effects are arranged in table:

– in the intra-block analysis the estimates are

i \ j	1	2	3	4
1	–	2.54	−1.96	2.24
2	−2.54	–	−1.36	1.27
3	1.96	1.36	–	0.62
4	−2.24	−1.27	−0.62	–

– in the inter-block analysis the estimates are

i \ j	1	2	3	4
1	–	1.66	−2.11	1.72
2	−1.66	–	−1.43	1.25
3	2.11	1.43	–	−0.12
4	−1.72	−1.25	0.12	–

Table 1. Statistical inferences

Hypotheses	F	P	F_o	P_o	z	$P(\chi^2_4 \mid H_o)$
1	42,048	10^{-19}	26,323	$3 \cdot 10^{-7}$	117,559	$2 \cdot 10^{-18}$
2	77,162	$4 \cdot 10^{-20}$	28,630	10^{-6}	116,764	$3 \cdot 10^{-18}$
3	133,137	$6 \cdot 10^{-42}$	121,025	$4 \cdot 10^{-15}$	256,392	$3 \cdot 10^{-40}$
$g_1 = 0$	38,094	$2 \cdot 10^{-8}$	45,343	10^{-6}	62,774	10^{-8}
$g_1 - g_2 = 0$	16,281	10^{-4}	39,375	$3 \cdot 10^{-6}$	43,436	$8 \cdot 10^{-9}$
$s_{12} = 0$	122,283	$3 \cdot 10^{-20}$	22,671	10^{-4}	135,310	$3 \cdot 10^{-25}$
$s_{12} - s_{13} = 0$	45,454	$2 \cdot 10^{-9}$	1,032	0,321	42,804	10^{-8}
$w_{12} = 0$	168,303	$2 \cdot 10^{-11}$	98,414	$2 \cdot 10^{-9}$	88,948	$2 \cdot 10^{-18}$
$w_{12} - w_{13} = 0$	264,130	$7 \cdot 10^{-12}$	253,802	$2 \cdot 10^{-11}$	100,389	$8 \cdot 10^{-21}$

– in the combined analysis the estimates are equal to those obtained in the intra-block analysis.

The comparison of the performances of the individual lines is of considerable interest for a plant breeder. Inferences on them can be made by testing the hypotheses 1–10, Table 1.

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Authors' address: Dr. Bronisław Ceranka and Dr. Stanisław Mejza, Academy of Agriculture in Poznań, Department of Mathematical and Statistical Methods, ul. Wojska Polskiego 28, 60–637 Poznań, Poland

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An algorithm for presenting pairs in optimum orders

W. G. Cloete*, I. Cloete** and K. von Gadow***

Summary

In 1934, R. T. Ross published tables for presenting pairs of stimuli in an optimum order. Ross's optimum order was characterized by two specifications:

a) maximum spacing: the number of pairs which appear between a first occurrence and every subsequent occurrence of the same pair element ist maximised

b) balance: an element in a pair appears as often on the right as on the left.

Zusammenfassung

Der Psychometriker R. T. Ross publizierte im Jahr 1934 eine Reihe von Tabellen für die optimale Anordnung von Paaren als Grundlage beim paarweisen Vergleich. Ross' optimale Anordnung, die zunehmend in der Praxis des Kriterienvergleichs angewendet wird, stützt sich auf zwei Maßstäbe:

a) maximaler Abstand: die Zahl der Paare zwischen einem ersten und jedem folgenden Erscheinen eines bestimmten Paar-Elementes sollte möglichst groß sein

b) Gleichgewicht: Jedes Paar-Element erscheint mit gleicher Häufigkeit auf der linken und rechten Seite.

Die vorliegende Arbeit beschreibt einen Algorithmus für die optimale Anordnung von Paaren nach Ross' Muster. Der Algorithmus, der auf der Graphentheorie basiert, läßt sich relativ einfach programmieren.

Ross' table are frequently being used in practical applications of pairwise comparisons. This article presents an algorithm for constructing Ross' oder in terms of complete graphs. The algorithm can be easily implemented on a computer.

Introduction

The assessment of judgmental information belongs traditionally to a branch of Psychology which is known as Psychometrics or Psychophysics. One of the most well-known Psychometric "laws" is Thurstone's Law of Comperative Judgement which is based on the assumption that relative preferences among different criteria ("stimuli") can be established if the criteria are lined up in pairs. One of the scientists who made an important contribution to the method of presenting pairs of stimuli in an optimum order was ROSS (1934, 1939). The method proposed by ROSS which is also being used in forestry (vide HULL, BUHYOFF and DANIEL, 1984), has the following characteristics:

1. An alternative is compared with every other alternative exactly once.
2. The pairs of alternatives are presented in a specific order. This order maximizes the number of pairs which appear between a first occurence und every subsequent occurence of the same alternative (ROSS' maximum spacing).
3. ROSS defines a characteristic, called balance, such that an alternative in a pair appears as often on the right as on the left.

ROSS did not give a formal mathematical development of his method. We shall construct ROSS' order in terms of complete graphs (CLOETE & CLOETE, in press).

An algorithm

First it is necessary to define a few graph-theoretic concepts. A complete graphs K_n is an ordered triple (V, E, ψ) consisting of a set V of vertices, E of edges (disjoint from V) and an incidence function ψ that associates with each edge of K_n two distinct vertices, such that there is an edge associated with every two distinct vertices (BONDY and MURTY, 1978). K_n has n vertices and thus $n(n-1)/2$ edges. We only consider the case where n is odd and $n \geq 5$. See figure 1 for a K_5 graph. Two edges which are incident with a common vertex are adjacent. A k-edge colouring of K_n is an assignment of k colours, $1, 2, \ldots, k$, to the edges of K_n. The colouring is proper if not two adjacent edges have the same colour. A proper k-edge colouring is a partition $(E_1, E_2, \ldots, E_k)$ of E, where E_i is a subset of E assigned colour i. The smallest number for which K_n has a proper edgecolouring is n.

Let an edge (v_1, v_2), where v_1 and v_2 are its vertices, represent a pair of alternatives v_1 and v_2. Owing to characteristic 1 it is clear that a complete graph is required when each pair in the ROSS order is represented by an unique edge.

In order to obtain maximum spacing (characteristic 2), find a maximum number of non-adjacent edges of K_n. That is, find subsets E_i of E with a maximum number of edges. This occurs in a proper n-edge colouring of K_n, where every E_i, $i = 1, \ldots, n$, has $(n-1)/2$ elements (BERGE, 1957). Thus maximum spacing is obtained within each E_i. Note that the E_i are

* Uitsigstr. 3, Stellenbosch
** Department of Electrical and Electronic Engineering
*** Department of Forest Science, University of Stellenbosch

Table 1. Table used for finding a proper n-edge colouring; for details see text

Column	1	2	3	m − 1	m
E_1	(m + 1, m + 3)	(m, m + 4)	(m − 1, m + 5)	(3, n)	(2, 1)
E_3	(m + 2, m + 3)	(m + 1, m + 5)	(m, m + 6)	(4, 2)	(3, 1)
E_5	(m + 3, m + 4)	(m + 2, m + 5)	(m + 1, m + 7)	(5, 3)	(4, 1)
E_7	(m + 4, m + 5)	(m + 3, m + 6)	(m + 2, m + 7)	(6, 4)	(5, 1)
E_{n-6}	(n − 3, n − 2)	(n − 4, n − 1)	(n − 5, n)	$\left(\frac{n-1}{2}, \frac{n-5}{2}\right)$	$\left(\frac{n-3}{2}, 1\right)$
E_{n-4}	(n − 2, n − 1)	(n − 3, n)	(n − 4, 2)	$\left(\frac{n+1}{2}, \frac{n-3}{2}\right)$	$\left(\frac{n-1}{2}, 1\right)$
E_{n-2}	(n − 1, n)	(n − 2, 2)	(n − 3, 3)	$\left(\frac{n+3}{2}, \frac{n-3}{2}\right)$	$\left(\frac{n+1}{2}, 1\right)$
E_n	(n, 2)	(n − 1, 3)	(n − 2, 4)	$\left(\frac{n+5}{2}, \frac{n-1}{2}\right)$	$\left(\frac{n+3}{2}, \frac{n+1}{2}\right)$
E_2	(2, 3)	(n, 4)	(n − 1, 5)	$\left(\frac{n+7}{2}, \frac{n+1}{2}\right)$	$\left(\frac{n+3}{2}, 1\right)$
E_4	(3, 4)	(2, 5)	(n, 6)	$\left(\frac{n+7}{2}, \frac{n+3}{2}\right)$	$\left(\frac{n+5}{2}, 1\right)$
E_6	(4, 5)	(3, 6)	(2, 7)	$\left(\frac{n+9}{2}, \frac{n+5}{2}\right)$	$\left(\frac{n+7}{2}, 1\right)$
E_8	(5, 6)	(4, 7)	(3, 8)	$\left(\frac{n+11}{2}, \frac{n+7}{2}\right)$	$\left(\frac{n+9}{2}, 1\right)$
E_{n-7}	(m − 2, m − 1)	(m − 3, m)	(m − 4, m + 1)	(n − 2, n − 4)	(n − 3, 1)
E_{n-5}	(m − 1, m)	(m − 2, m + 1)	(m − 4, m + 2)	(n − 1, n − 3)	(n − 2, 1)
E_{n-3}	(m, m + 1)	(m − 2, m + 2)	(m − 3, m + 3)	(n, n − 2)	(n − 1, 1)
E_{n-1}	(m, m + 2)	(m − 1, m + 3)	(m − 2, m + 4)	(2, n − 1)	(n, 1)

ordered sets. However, an ordered sequence of the E_i such that maximum spacing is also maintained in the overall order, is required. For an E_i, i = 1, . . ., n, there is exactly one vertex, say v_i, where $v_i \notin V_i$, the vertex-set of E_i, but $v_i \in V_j$, $\forall\, j \neq i$. To construct an overall order with maximum spacing this v_i is used as a vertex of the first edge of E_{i+1}, i = 1, . . ., n−1.

An algorithm to construct the Ross order is presented. Let m = (n−1)/2. We label the vertices of K_n using the numbers 1, . . ., n. The algorithm consists of three steps:

(a) Find a proper n-edge colouring by means of table 1. The rows of table 1 give the subsets E_i of the partition. Each entry is an edge (v_i, v_j) of K_n. Construct the partition using table 1 as follows:

1. Select the first m-1 columns as well as the last column, and the first m rows, the middle row (with colour n) as well as the last m rows. This defines an n by m matrix of edges.
2. Now consider the first m-1 columns and all n rows, and for every vertex

   if $v_i > n$ then let $v_i = (1+v_i) \bmod_n$ or
   if $v_i < 2$ then let $v_i = n-1+v_i$.

(b) Pack the resulting edges to obtain the final ordering by means of table 2 which contains the position number of the corresponding edge found in table 1.

(c) Balance the vertices to satisfy characteristic 3. Note for n odd it is always possible to achieve perfect balance (CLOETE & CLOETE, in press).

A computer algorithm is implemented in Pascal (JENSEN and WIRTH, 1974)*.

It is clear that the ROSS order for any n is not unique because K_n has a number of proper n-edge colourings. For K_5, for example, we can give three orders which satisfy the characteristic of maximum spacing:

(2,1), (5,3), (1,4), (3,2), (4,5), (1,3), (2,5), (3,4), (5,1), (4,2);
(2,1), (3,5), (4,2), (1,3), (5,4), (3,2), (5,1), (4,3), (2,5), (1,4);
(1,2), (5,3), (4,1), (2,5), (3,4), (1,5), (4,2), (3,1), (5,4), (2,3).

Note that there are proper n-edge colourings which do not satisfy the characteristic of maximum spacing.

An example

Suppose we are given the task to set the priorities in a silvicultural research programme, involving the following 5 major fields of research:

Forest Ecology, Soils & Climate	(1)
Species Trials and Tree Breeding	(2)
Applied Silviculture	(3)
Forest Protection	(4)
Scientific Services (Biometry)	(5)

Table 2. Table used for packing edges; for details see text

	Column					
	1	2	3	m − 2	m − 1	m
E_1	m	m − 1	m − 2	3	2	1
E_3	1	m	m − 1	4	3	2
E_5	2	1	m	5	4	3
E_{n-4}	m − 2	m − 3	m − 4	1	m	m − 1
E_{n-2}	m − 1	m − 2	m − 3	2	1	m
E_n	m	m − 1	m − 2	3	2	1
E_2	2	3	4	m − 1	m	1
E_4	3	4	5	m	1	2
E_6	4	5	6	1	2	3
E_{n-5}	m − 1	m	1	m − 4	m − 3	m − 2
E_{n-3}	m	1	2	m − 3	m − 2	m − 1
E_{n-1}	1	2	3	m − 2	m − 1	m

* Information about the programme by I. CLOETE

The 5 criteria are lined up in $n(n-1)/2 = 10$ Pairs, which are represented by the K_5 graph. Every E_i consists of 2 edges (with the same colour) and there are 5 ordered colourses, given by

$E_1 = \{ (1,2), (5,3) \}$
$E_2 = \{ (4,1), (3,2) \}$
$E_3 = \{ (4,5), (1,3) \}$
$E_4 = \{ (2,4), (5,1) \}$
$E_5 = \{ (3,4), (2,5) \}$

which is the ROSS pairing for n = 5:

(1,2), (5,3), (4,1), (3,2), (4,5),
(1,3), (2,4), (5,1), (3,4), (2,5)

obtained from the computer algorithm. The resulting colouring is illustrated in figure 1.

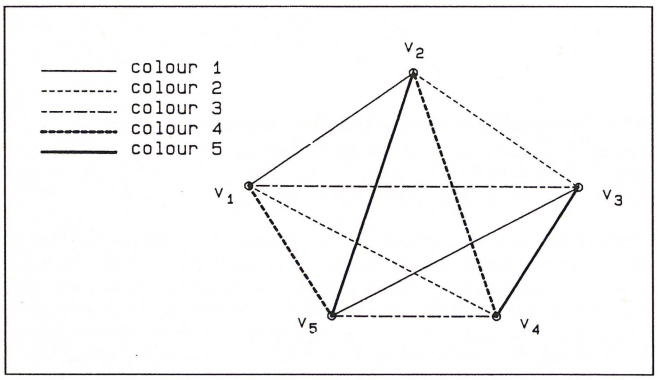

Fig. 1. Edge-colouring for n = 5

The set of pairs is presented in Table 3.

Standard methods are available for evaluating a particular assessment (VON GADOW, 1986), but we will not discuss these here.

Remarks

Many decisions are taken on the basis of foresters' personal perception of things. Mathematical models for the description of mental phenomena can be used to capture personal preferences.

The method of paired comparisons, using ROSS' optimal ordering of pairs, is a useful procedure for presenting criteria for assessment. The graph-analytic algorithm proposed in this paper can be easily implemented on a computer and this is convenient, especially if n is large. There is mathematical proof that ROSS' empirical spacings are optimal, though not uniquely optimal.

Table 3. Example of a set of balanced pairs and completed assessment

How do you rate the relative importance of X against Y?

X	Assessment			Y
	more important	equally important	less important	
ecology		*		breeding
services	*			applied
protection		*		ecology
applied	*			breeding
protection			*	services
ecology		*		applied
breeding	*			protection
services	*			ecology
applied		*		protection
breeding	*			services

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Anschrift der Autoren: W. C. Cloete und I. Cloete, Uitsigstr. 3, 7600 Stellenbosch, Südafrika. K. v. Gadow, Department of Forest Science, Faculty of Forestry, University of Stellenbosch, 7600 Stellenbosch, Südafrika

BUCHBESPRECHUNGEN/BOOK REVIEWS

FORD, N.
So denken Maschinen
Einführung in die Künstliche Intelligenz am Beispiel von PROLOG
1988, 242 S., DM 48.–
R. Oldenburg Verlag, München – Wien

Der Einstieg in das Gebiet der künstlichen Intelligenz ist besonders für Nicht-Computerfachleute oft problematisch. Häufig trägt die intensive Beschäftigung mit den komplexen Programmierprinzipien, die zur Nachahmung menschlicher Denkvorgänge angewandt werden, eher zur Verwirrung als zur Aufklärung desjenigen bei, der sich praktisch anwendbare Kenntnisse über künstliche Intelligenz (KI) aneignen will.

Das Buch „So denken Maschinen" bildet hier eine Ausnahme. Es zielt darauf ab, Leser ohne tiefergehende mathematische und wissenschaftliche Vorkenntnisse mit den wichtigsten KI-Konzepten vertraut zu machen. Die Einzelheiten der Programmierung werden in PROLOG angegeben, und zwar in einer weithin akzeptierten Grundversion dieser KI-Sprache, deren Beliebtheit auf der ganzen Welt ständig zunimmt. Daneben findet der Leser jedoch die Übersetzung der Programme in gewöhnlicher Sprache, so daß er das Buch parallel in beiden „Sprachen" lesen kann. Mit Hilfe von verschiebbaren Programmkarten werden dem Leser einige wichtige Programmierkonzepte anschaulich gemacht, und er kann den Ablauf der Programme plastisch nachvollziehen. Das Buch beschreibt auf einfache Weise zahlreiche komplexe Systeme aus der Praxis, die eindrucksvolle Ergebnisse liefern. Es schließt mit einer klaren, prägnanten Diskussion der philosophischen Fragen, die sich im Zusammenhang mit den Versuchen stellen, Computer mit „Intelligenz" auszustatten. Ge.

FAULBAUM, F. u. UEHLINGER, H.-M. (Hrsg.)
Fortschritte der Statistik-Software 1
4. Konferenz über die wissenschaftliche Anwendung von Statistik-Software, Heidelberg 1987
1988, 595 S., DM 76,–
Gustav Fischer Verlag, Stuttgart – New York

Unter internationaler Beteiligung fand in Heidelberg vom 23. –26. März 1987 die 4. Konferenz über die wissenschaftliche Anwendung von Statistik-Software statt.

Die Situation auf dem Gebiet der Anwendung von Statistik-Software wird heute geprägt durch die rasche Entwicklung leistungsfähiger PCs, die Einbeziehung von Hochleistungsgraphik in die statistische Datenanalyse, die Bemühungen um immer größere Benutzerfreundlichkeit sowie die Tendenz zur Expansion der großen Statistikpakete einerseits und zur individuellen statistischen Modellierung andererseits. Die in den 60 Referaten dieses Konferenzbandes angesprochenen Themen spiegeln die gegenwärtige Situation wider und informieren über sich andeutende Entwicklungen. Ge.

SAVORY, S. E.
Grundlagen von Expertensystemen
Ein Lehrbuch der Nixdorf Computer AG
1988, 276 S., DM 48,–
R. Oldenbourg Verlag, München – Wien

„Ein Ziel dieses Buches ist, daß alle Leser anschließend Expertensysteme erstellen oder zumindest verstehen können und lernen, was alles damit gemacht werden kann." Trotz vieler Zitate wird dieses Ziel wohl nur teilweise erreicht. Wenn beispielsweise dem Lernen durch Beispiele auch viel Raum gewidmet wurde, so wären doch an vielen Stellen konkrete Beispiele besser als die Auflistung von Möglichkeiten.

Insgesamt hat das vorliegende Buch mehr den Charakter eines Handbuches, das dem Leser einen nützlichen Einstieg in dieses Gebiet ermöglicht. Ge.

MERTEN, K.
FORTRAN 77
3. Aufl., UTB 428
1988, 290 S., DM 29,80
Gustav Fischer Verlag, Stuttgart

Die Programmiersprache FORTRAN hat immer noch ihre Bedeutung, nur erwartet man heute von einer ausdrücklich für Anfänger geschriebenen Einführung zum Selbststudium eine den heutigen Rechenmöglichkeiten angepaßte Darstellung. Die Verwendung von Lochkarten gehört der Vergangenheit an. Von daher sollte mehr der Dialogverarbeitung sowie der Benutzung von Standardsoftwarepaketen Rechnung getragen werden. Eine Anzahl von Ungenauigkeiten in der Darstellung sollte bei einer weiteren Auflage korrigiert werden. Ge.

MEIER, F. (Hrsg.)
Prozeßforschung in den Sozialwissenschaften
Anwendung zeitreihenanalytischer Methoden
1988, 174 S., DM 58.–
G. Fischer Verlag, Stuttgart – New York

Obwohl die Analyse von Zeitreihen mittlerweile einen festen Platz in den Sozialwissenschaften gefunden hat, zählt die Prozeßforschung wohl auch aufgrund des erhöhten Untersuchungsaufwandes und der komplexen Analysemethoden noch immer zu den eher randständigen Forschungsstrategien und ist weit entfernt von einer standardmäßigen Anwendung. Der vorliegende Band bietet daher zur Anregung einen aktuellen interdisziplinären Querschnitt prozeßanalytischer Untersuchungsansätze bzw. Anwendungsbeispiele aus Bereichen der Politikwissenschaften, Soziologie, Sozialmedizin, Sozialpsychologie und arbeitswissenschaftlichen Beanspruchungsforschung.

Inhaltsübersicht: Krieg und Regierungspopularität: Der Fall der Falklands – Interventionsanalyse: Anwendung der BOX-JENKINS-Methode zur Evaluation einer legislativen Maßnahme – Ein Evaluationsproblem in der Suizidforschung aus prozeßanalytischer Sicht – Modelle zur Analyse qualitativer Variablen in stetigem Zeitverlauf – Parameteraggregation individueller Zeitreihenschätzung – Ein Verfahren zur dynamischen Analyse dyadischer Interaktionen. Ge.

NACHRICHTEN UND BERICHTE

Second Conference of the International Federation of Classification Societies (IFCS)

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If you plan to present a paper, send an English abstract of at most one page to: Robert F. Ling, Chairman, IFCS-89 Program Committee, Dept. of Math. Sciences, Clemson Univ., Clemson, SC 29634-1907, or (Bitnet: RFLING & CLEMSON). Deadline for submitting papers is January 15, 1989.

SCHADSTOFFBELASTUNGEN IN ÖKOSYSTEMEN UND IHRE ERFASSUNG

Dieses Werk geht auf eine Studie „Bioindikatoren zur Beurteilung von Schadstoffbelastungen der Umwelt“ zurück, die im Jahre 1979 im Institut für Landeskultur und Pflanzenökologie der Universität Hohenheim im Auftrag des Umweltbundesamtes durchgeführt wurde. In den Jahren 1985 und 1986 wurde eine Aktualisierung und eine umfassende Überarbeitung vorgenommen. Nunmehr bilden nahezu 1000 Literaturzitate, deren Schwerpunkt europäisch ist, die Basis dieses Buches. Es wendet sich an Bundes- und Landesbehörden, die sich mit Fragen des Umweltschutzes befassen, an Immissionsschutzbeauftragte und Technische Überwachungsvereine, und kann als → **kritische Literaturübersicht** auch von wissenschaftlichen Instituten verwendet werden. Es bringt beispielsweise Hinweise für die → **Planung und den Aufbau von Umweltprobenbanken,** für die Entwicklung von Prüfverfahren für Umweltchemikalien und für die Einrichtung und den Betrieb von Wirkungskatastern. Die Form der Zusammenfassung und Gruppierung von Bioindikatoren erlaubt auch dem weniger in der Materie vertrauten Leser, einen schnellen Überblick zu erhalten. Aus den Tabellen lassen sich bequem sowohl Hinweise für die Umsetzung wissenschaftlicher Erkenntnisse in → **Maßnahmen des praktischen Umweltschutzes** entnehmen als auch Anregungen bei der sinnvollen Vergabe von Forschungsvorhaben zur Entwicklung weiterer Bioindikatoren gewinnen. **Bioindikatoren.** Möglichkeiten, Grenzen und neue Erkenntnisse. Von → **Prof. Dr. Uwe Arndt, Dr. Willfried Nobel und Birgit Schweizer,** alle Stuttgart. 396 Seiten mit 36 Farbfotos, 139 Abb. und 102 Tab. Kst. → **DM 68,–.**

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